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RESEARCH AND DEVELOPMENT TECHNICAL REPORT
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TEMPERATURE AND COUPLING BEHAVIOR OF RESONATORS AND TRANSDUCERS OF LITHIUM TETRABORATE DRIVEN BY LATERAL AND THICKNESS FIELDS

ARTHUR BALLATO, JOHN KOSINSKI, MUHAMMAD MIZAN, AND THEODORE LUKASZEK

ELECTRONICS TECHNOLOGY AND DEVICES LABORATORY

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Lithium tetraborate is a tetragonal material of considerable promise for signal processing, transducer, and frequency control applications. It exhibits piezoelectric coupling values that fall between those of lithium niobate and quartz, but possesses orientations for which the temperature coefficient of frequency or delay time is zero for both bulk and surface acoustic waves.

Calculations have previously been made for rotated y-cut, bulk wave plates, including the regions where the quasi-extensional and quasi-shear thickness modes have zero temperature coefficients of frequency. In this report we extend the calculations to doubly rotated bulk wave resonators, and compute the coupling factors for the three simple thickness modes driven by [TE] and lateral [LE] quasistatic electric fields as a function of the orientation angles phi and theta, and the direction of the applied lateral field psi. Because of the temperature coefficients of the piezoelectric coupling factors, the temperature coefficient (contd)

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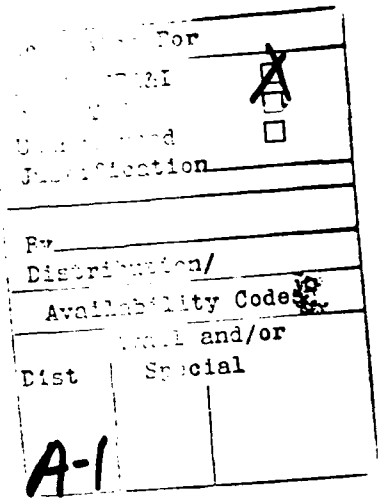
of a resonator will depend not only upon orientation, but also upon harmonic number and location of the resonator operating point on the immittance circle.

It is found that two unique orientations exist in lithium tetraborate for which plate resonators have zero temperature coefficients of frequency of both first- and second-order with high values of piezo coupling factor. One cut has this favorable behavior in its thickness-stretch mode, while the other possesses it for its slow thickness-shear mode.



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INTRODUCTION

Lithium tetraborate (LBO) is a tetragonal material in crystal class 4mm (C_{4v}). As such it possesses a single 4-fold polar axis, and four symmetry planes containing the 4-fold axis; consequently, there are 6 independent linear elastic constants, three independent linear piezoelectric constants, and two independent linear dielectric constants.

The primitive region is 1/8th of a hemisphere, which we comprise as the angle ranges (yxwl)Φ/Θ, with $0 \leq \Phi \leq \pi/4$ and $0 \leq \Theta \leq \pi/2$. As a consequence of its symmetry, LBO is

- Pyroelectric
- Optically uniaxial (LBO is negative)
- Piezoelectric
- Not enantiomorphic (no twinning)
- Nonferroelectric (poling not required)

Particularizing to the substance lithium tetraborate (LBO), we find from the literature [1]-[26], [30]-[32], the following specific properties and virtues:

Properties of $Li_2B_4O_7 = Li_2O \cdot 2B_2O_3$

- Congruently melting phase in the lithium oxide-boron oxide system; transparent and colorless.
- Low melting point: 917°C.
- Czochralski growth, Pt crucibles, diameters > 50 mm along [100], [001], or [110]; sensitive to thermal shock (cooling).
- Lattice spacings: a = b = 9.479 Å, c = 10.280 Å.
- Mohs hardness = 6 (between $LiTaO_3$ and quartz = 7).
- Low density = 2451 kg/m^3, but acoustic velocities only slightly greater than those in $LiNbO_3$ and $LiTaO_3$.
- Solubility: 1) dissolves rapidly in acids, slowly in bases. 2) hot water used as etchant. 3) insolvent in organic "solvents."
- Relatively high piezocoupling k and $\underline{k}$ values.
- Surface acoustic wave (SAW) reflectivity per stripe > 5 times that for $LiNbO_3$, $LiaO_3$, and quartz, leading to miniaturization.
- Zero temperature coefficients of frequency and time delay for BAW and SAW.

DETERMINATION OF CONSTANTS

The elastic, piezoelectric, and dielectric constants of 4mm crystals may be determined from the simple thickness modes of thin plates driven by thickness excitation [TE] and lateral excitation [LE].

Orientation (yx); Y-cut = X-cut

[TE]: pure shear along X_3
c_{44}^E, e_{15}, ϵ_{11}^S

[LE]: pure stretch along X_2, driven by X_3 field
c_{11}^E, e_{31}

Orientation (zx); Z-cut

[TE]: pure stretch along X_3
c_{33}^E, e_{33}, ϵ_{33}^S

Orientation (yxl)θ; rotated Y-cut

[TE]: coupled shear-stretch
c_{13}^E
[LE]: pure shear along X_1, driven by X_1 field
c_{66}^E

Orientation (yxw)Φ

[LE]: coupled shear-stretch, field along X_3; X_1, X_2 motion
c_{12}^E

COMPUTATIONAL SCHEME

Input data are taken from Ref. [19], and used as follows:

- s^E, d, ϵ^T are converted to c^E, e, ϵ^S.
- c^E, e, ϵ^S, density, and thickness are given at reference temperature T_o = 25°C.
- First- and second-order temperature coefficients TC(1) and TC(2) are used to compute c^E, etc., at two other temperatures, T_c and T_h.
- For assumed angles Φ,θ, and psi, the conventional eigenvalue problem is solved to yield N_m, k_m, $\underline{k}_m$(psi), etc., for each temperature, T_c, T_o, and T_h.
- TC(1) and TC(2) of f_R, f_A, etc., are computed for each mode, harmonic, and excitation type; for further details, see Refs. [27]-[29].

FREQUENCY CONSTANTS AND COUPLING FACTORS

The frequency constants, N_m, [TE] coupling factors, k, and [LE] coupling factors, $\underline{k}$(psi), for (yxwl)Φ=0°(15°)45°/θ cuts having applied field direction psi = 0°(30°)90°, are given in Figs. 1 to 24, respectively.

TEMPERATURE COEFFICIENTS

The first- and second-order temperature coefficients of frequency, TC(1) and TC(2), and the loci of TC(1)=0 and TC(2)=0, for M = 1, 3, and ∞, for [TE] (yxwl)Φ=0°/θ plates are given, respectively, for the "a" mode in Figs. 25 to 28, for the "b" mode in Figs. 29 to 32, and for the "c" mode in Figs. 33 to 36.

The first- and second-order temperature coefficients of frequency, TC(1) and TC(2), and the loci of TC(1)=0 and TC(2)=0, for mode "a", psi=0°(30°)90°, for [LE] (yxwl)Φ=0°/θ plates are given, respectively, for M=1 in Figs. 37 to 40, for M=3 in Figs. 41 to 44, and for M=∞ in Figs. 45 to 48.

The first- and second-order temperature coefficients of frequency, TC(1) and TC(2), and the loci of TC(1)=0 and TC(2)=0, for mode "b", psi=0°(30°)90°, for [LE] (yxwl)Φ=0°/θ plates are given, respectively, for M=1 in Figs. 49 to 52, for M=3 in Figs. 53 to 56, and for M=∞ in Figs. 57 to 60.

The first- and second-order temperature coefficients of frequency, TC(1) and TC(2), and the loci of TC(1)=0 and TC(2)=0, for mode "c", psi=0°(30°)90°, for [LE] (yxwl)Φ=0°/θ plates are given, respectively, for M=1 in Figs. 61 to 64, for M=3 in Figs. 65 to 68, and for M=∞ in Figs. 69 to 72.

COMPENSATED, DOUBLY ROTATED CUTS

Superposition of Figs. 27 and 28 discloses that a unique doubly rotated "a" mode orientation in LBO exists for which TC(1) = TC(2) = 0. It occurs for Φ/θ ≈ 40°/33° at the fundamental harmonic, driven in [TE]. In a plate resonator or transducer cut at this orientation, both TC(1) and TC(2) are zero. This means that the first surviving temperature coefficient will be TC(3); i.e., the frequency-temperature curve will be cubic in nature, like that of the AT and SC cuts of quartz, and the overall excursions in frequency over a wide temperature range will be small. The corresponding N_a and k_a values may be read approximately from the graphs in Figs. 19 and 20, respectively. The frequency constant N_a is nearly a maximum when θ ≈ 33°, and the piezocoupling factor k_a is approximately 20%.

Superposition of Figs. 35 and 36 discloses that a unique doubly rotated "c" mode orientation in LBO also exists for which TC(1) = TC(2) = 0. It occurs for Φ/θ ≈ 19°/56° at the fundamental harmonic, driven in [TE]. In a plate resonator or transducer cut at this orientation, both TC(1) and TC(2) are likewise zero. This again means that the first surviving temperature coefficient will be TC(3); i.e., the frequency-temperature curve will be cubic in nature, like that of the AT and SC cuts of quartz, and the overall excursions in frequency over a wide temperature range will be small. The corresponding N_a and k_a values may be read approximately from the graphs in Figs. 7 and 8, respectively. The frequency constant N_a is nearly a minimum when θ ≈ 56°, and the piezocoupling factor k_a is approximately 27%.

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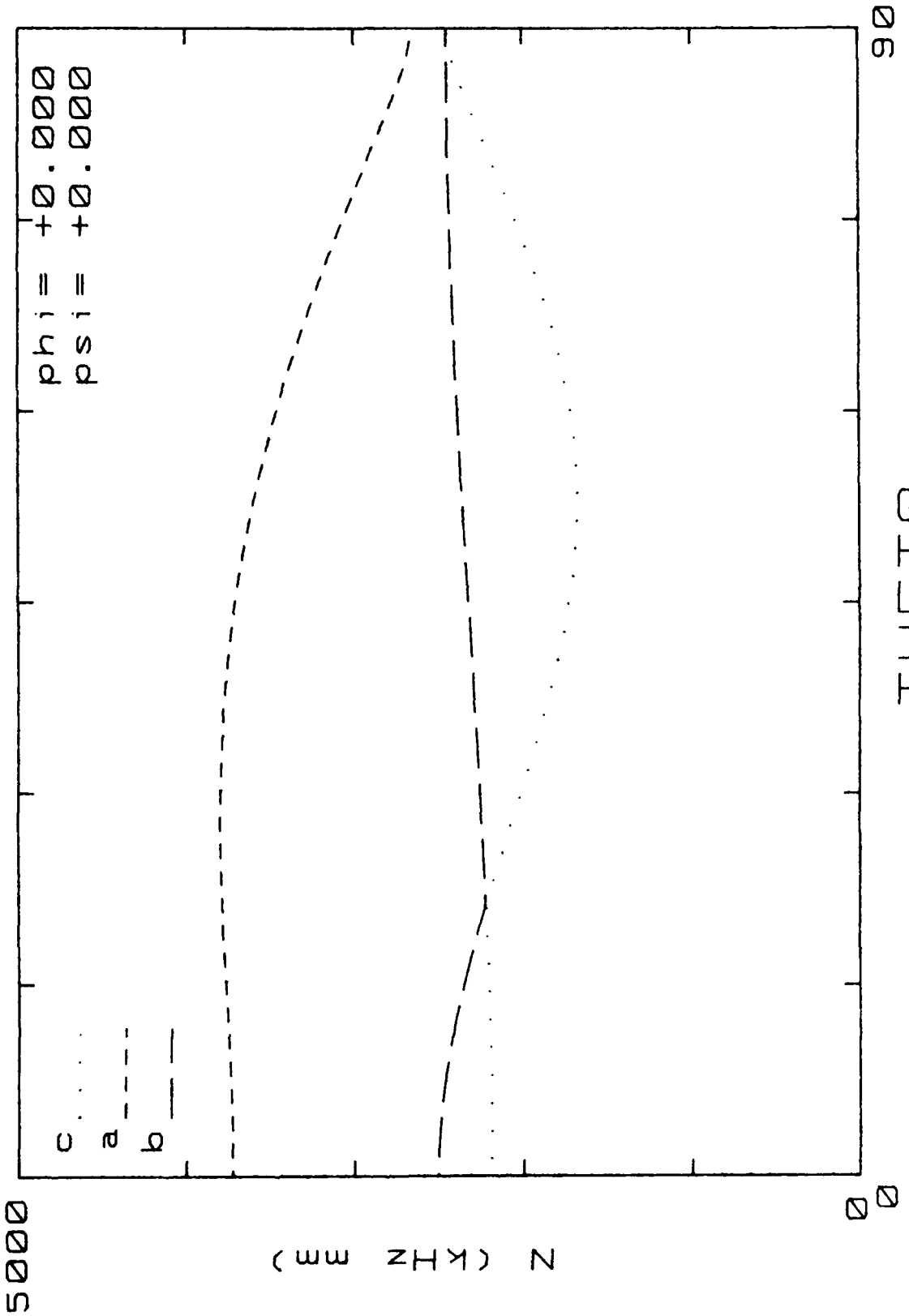


Figure 1. Frequency constant, N_m, for (yxwl)ϕ =0°/θ cuts.

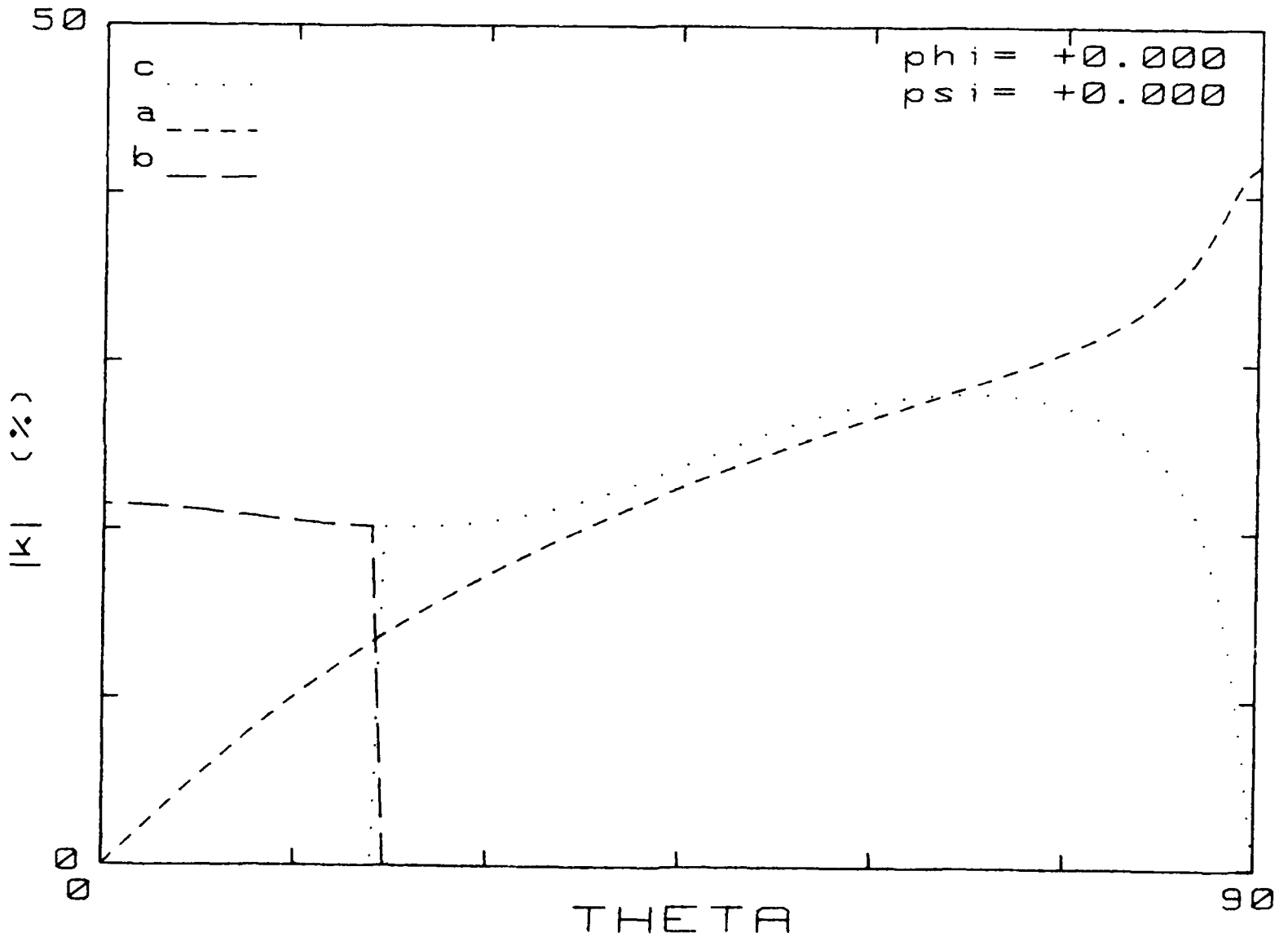


Figure 2. Piezocoupling, k_m, for (yxwl)ϕ =0°/θ cuts.

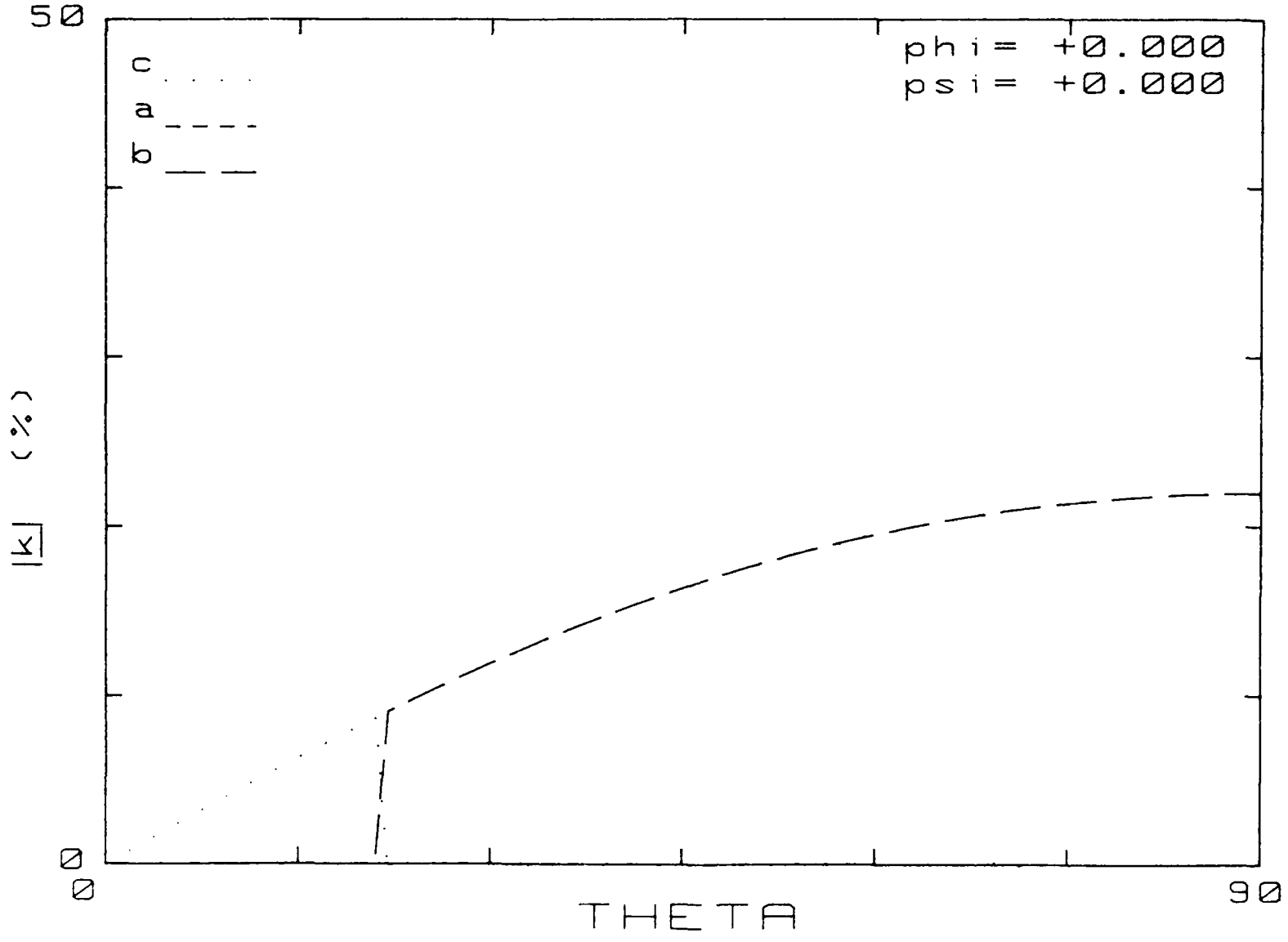


Figure 3. Piezocoupling, $\underline{k}_m$, for (yxwl)ϕ =0°/θ, psi=0° cuts.

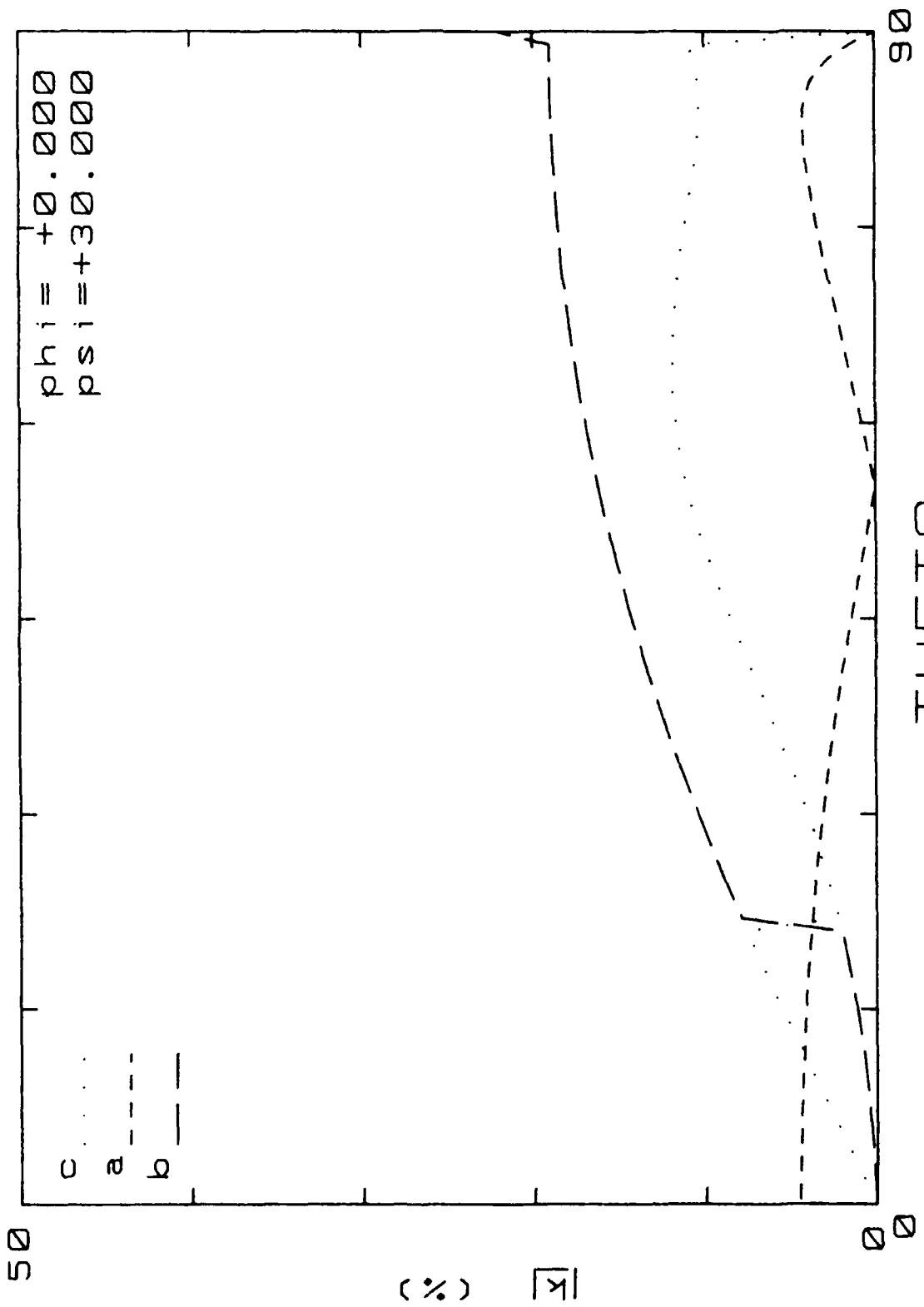


Figure 4. Piezocoupling, k_m, for (yxwl)ϕ=0°/θ, psi=30° cuts.

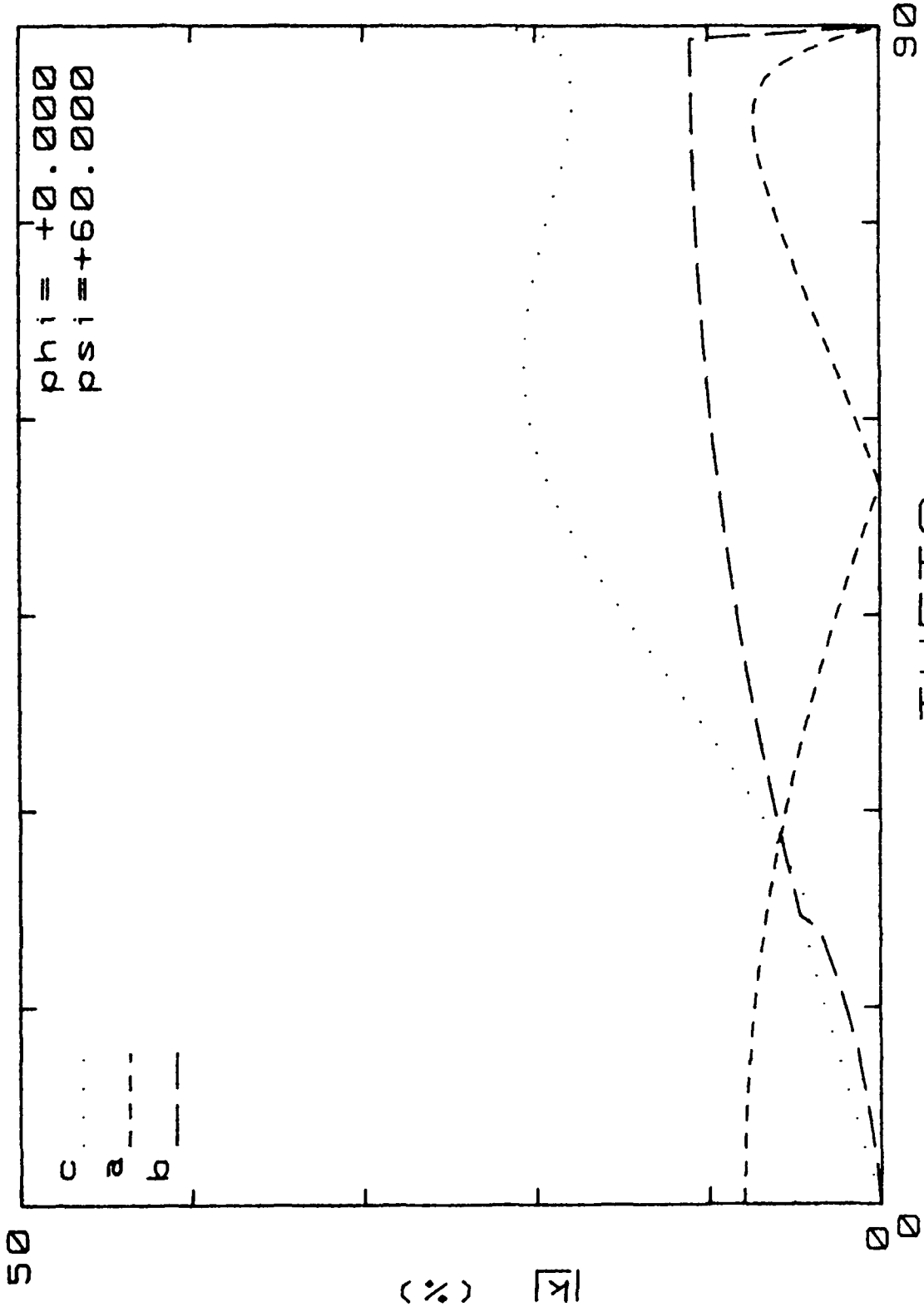


Figure 3. Piezocoupling, k_m, for (yxwl)ϕ=0°/θ, psi=60° cuts.

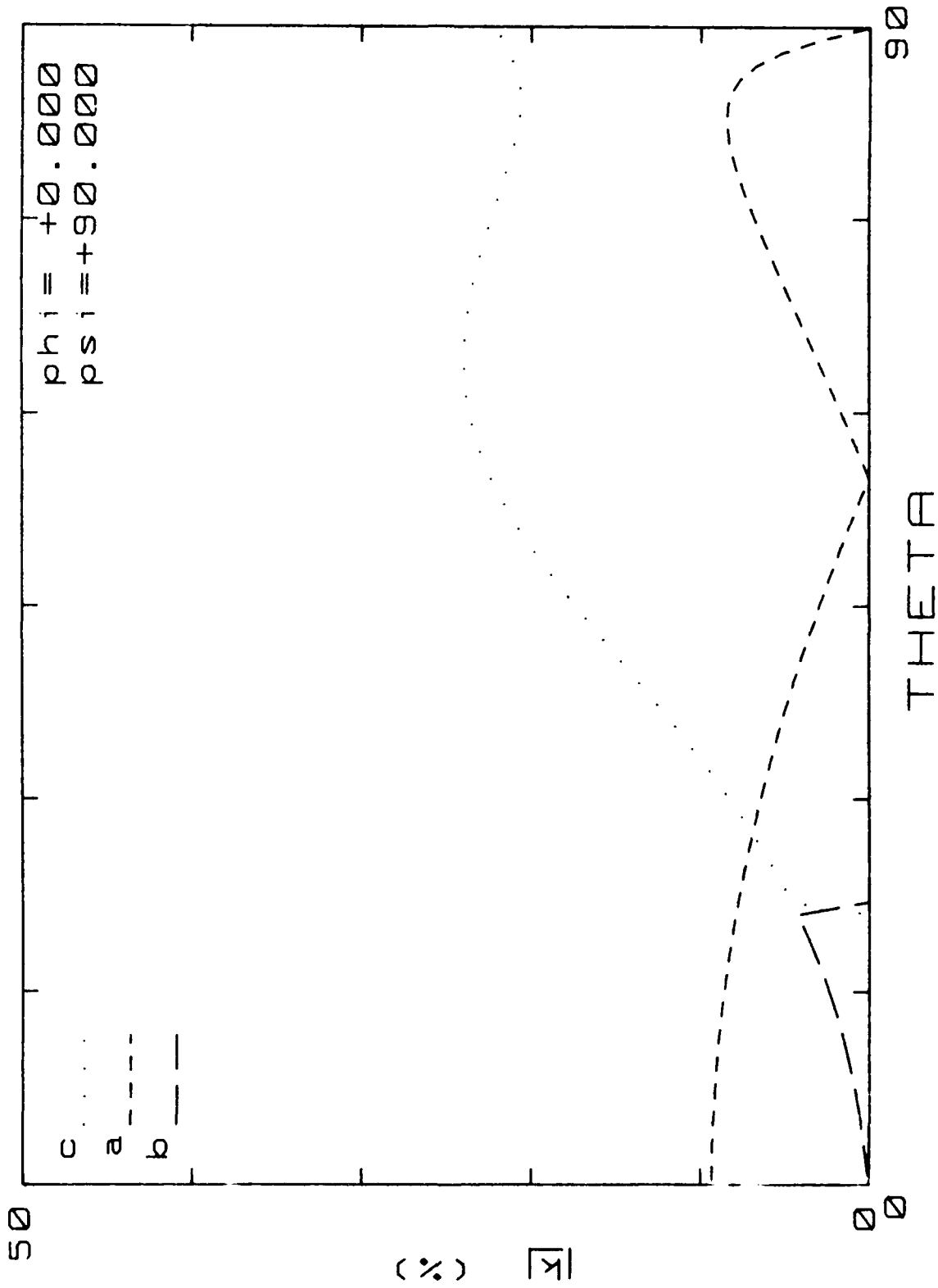


Figure 6. Piezocoupling, k_m, for (yxwl)ϕ=0°/θ, psi=90° cuts.

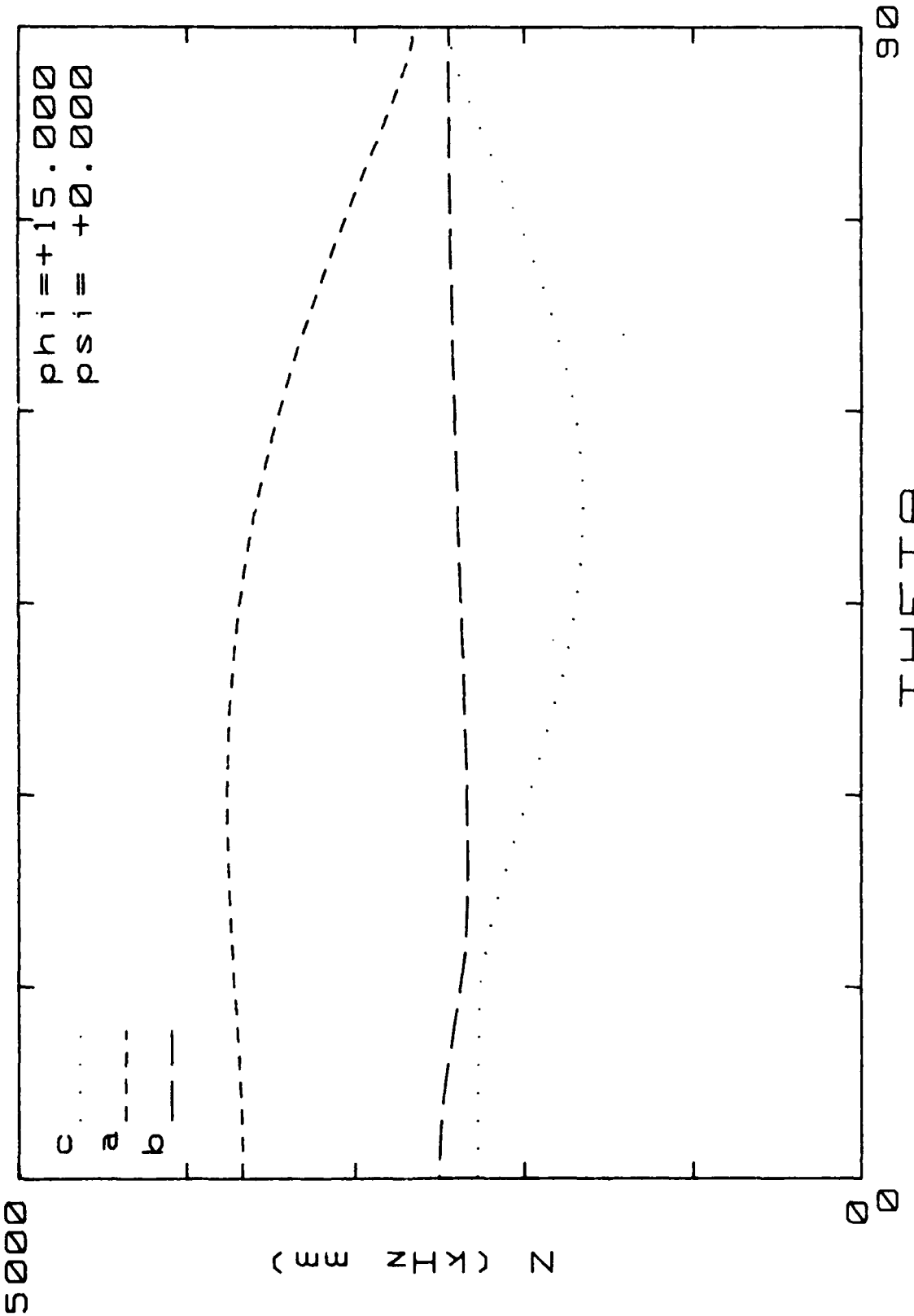


Figure 7. Frequency constant, N_m, for (yxwl) ϕ=15°/θ cuts.

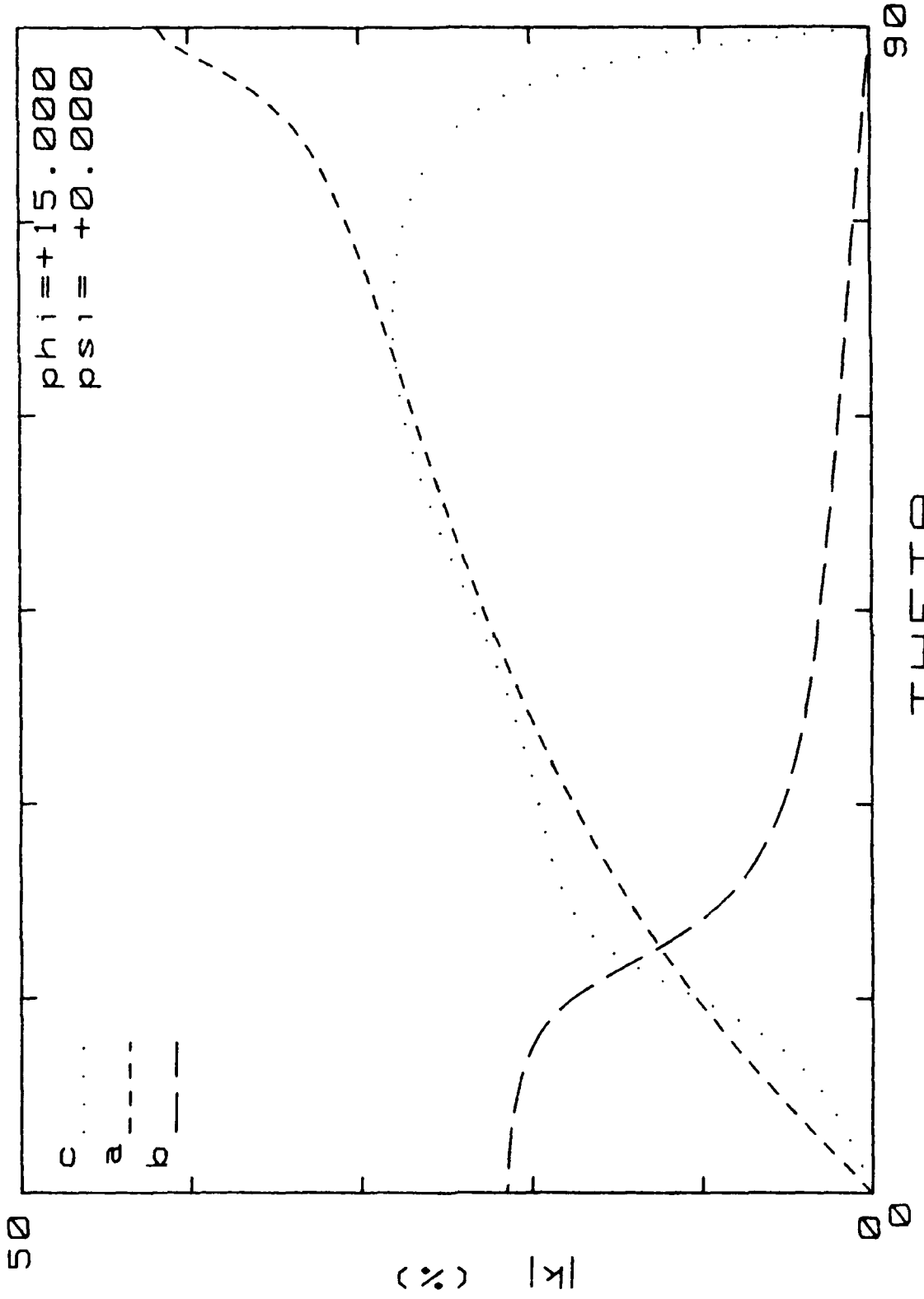


Figure 8. Piezocoupling, k_m, for (yxwl)ϕ=15°/θ cuts.

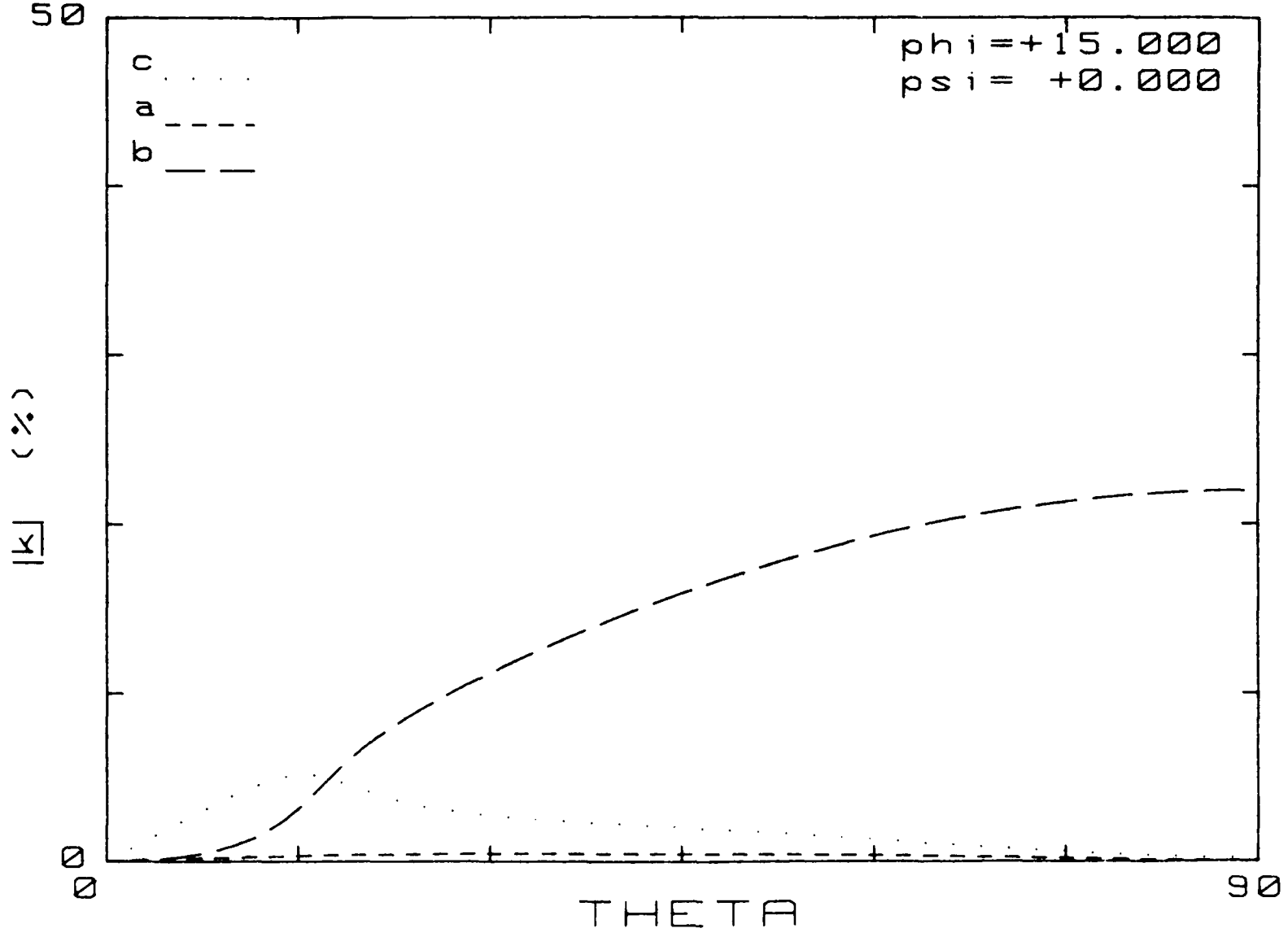


Figure 9. Piezocoupling, $\underline{k}_m$, for (yxwl)ϕ =15°/θ, psi=0° cuts.

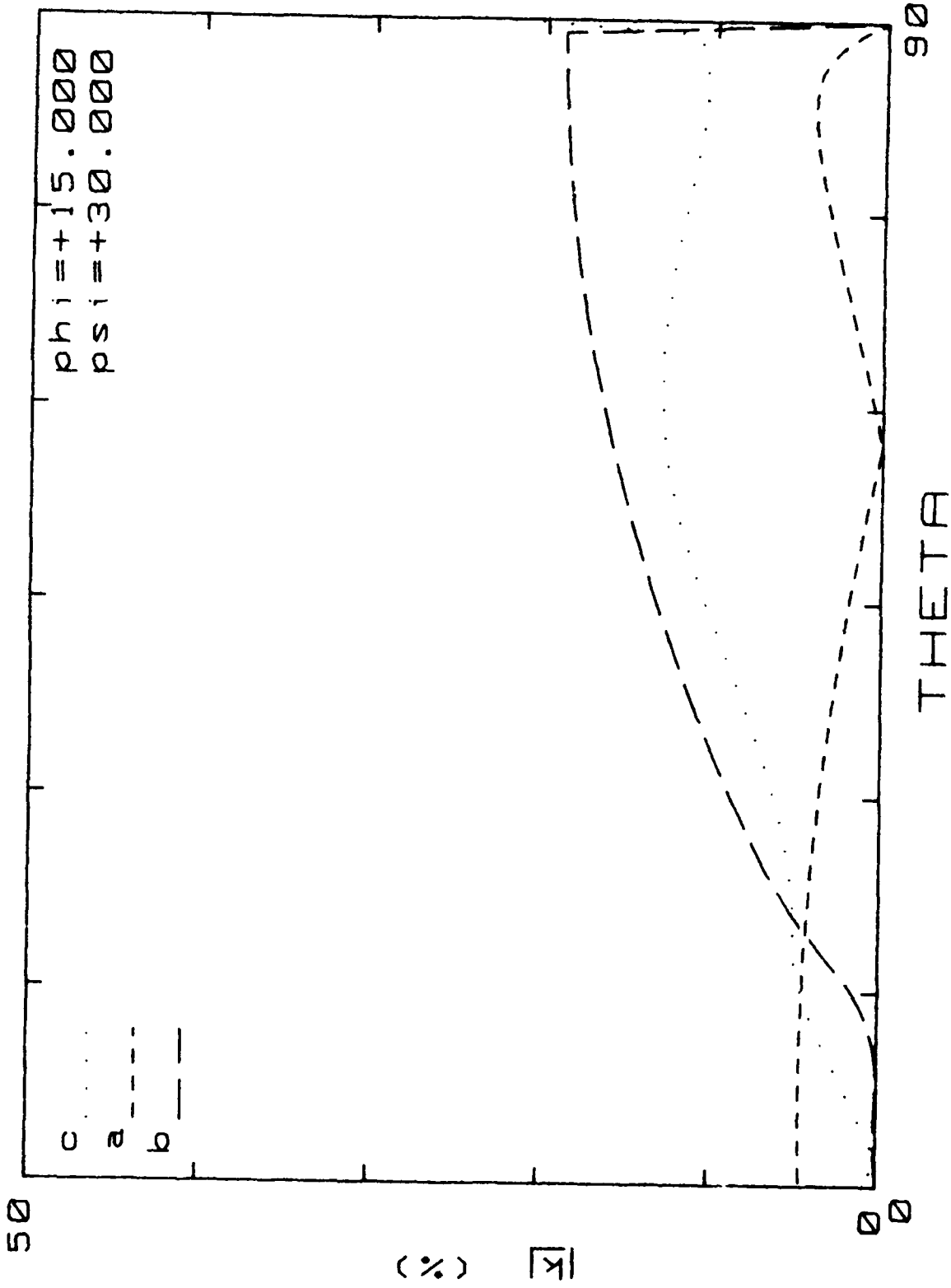


Figure 10. Piezocoupling, k_m, for (yxwl)ϕ =15°/θ, psi=30° cuts.

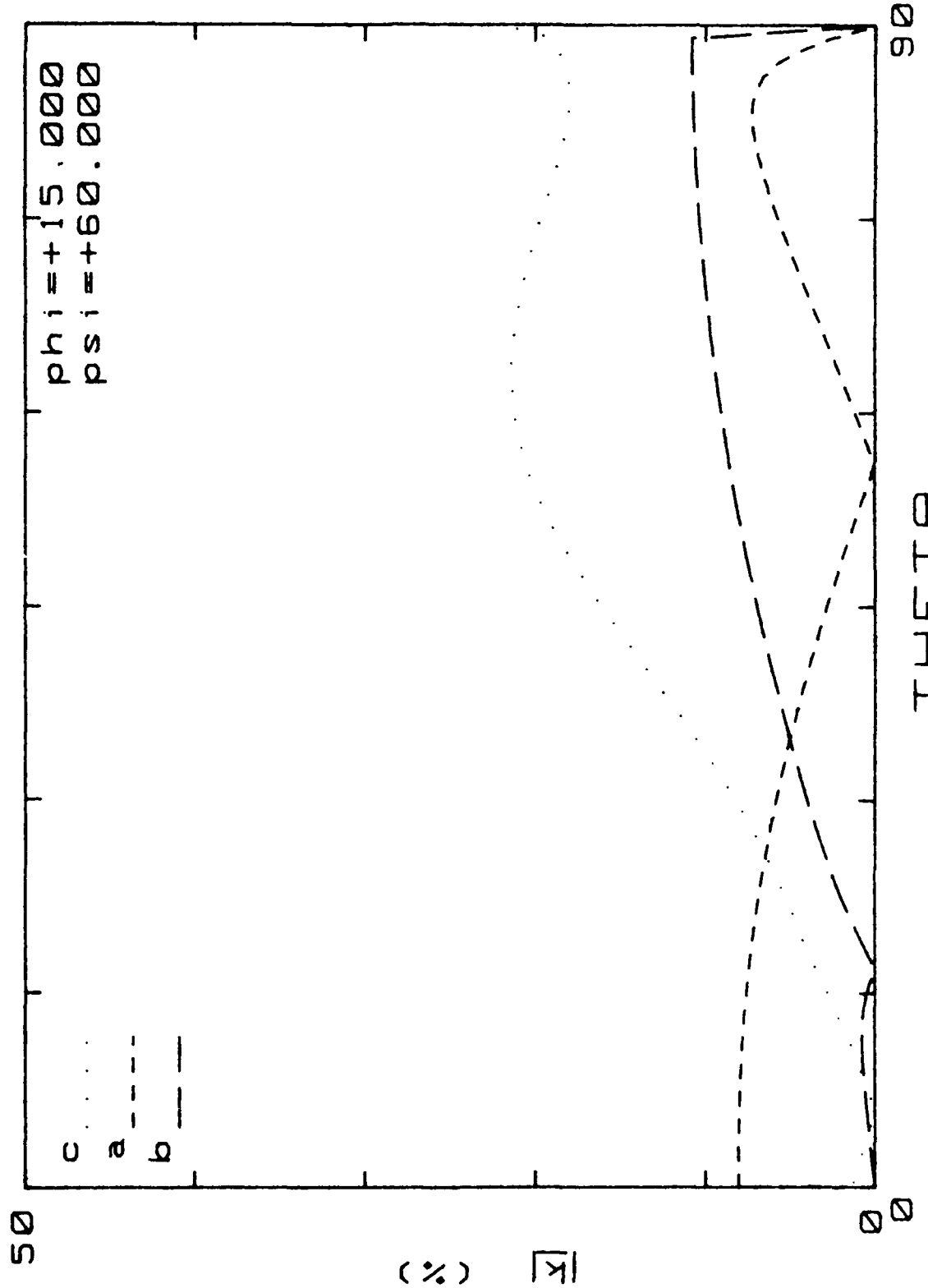


Figure 11. Piezocoupling, k_{fm}, for (yxwl)ϕ=15°/θ, psi=60° cuts.

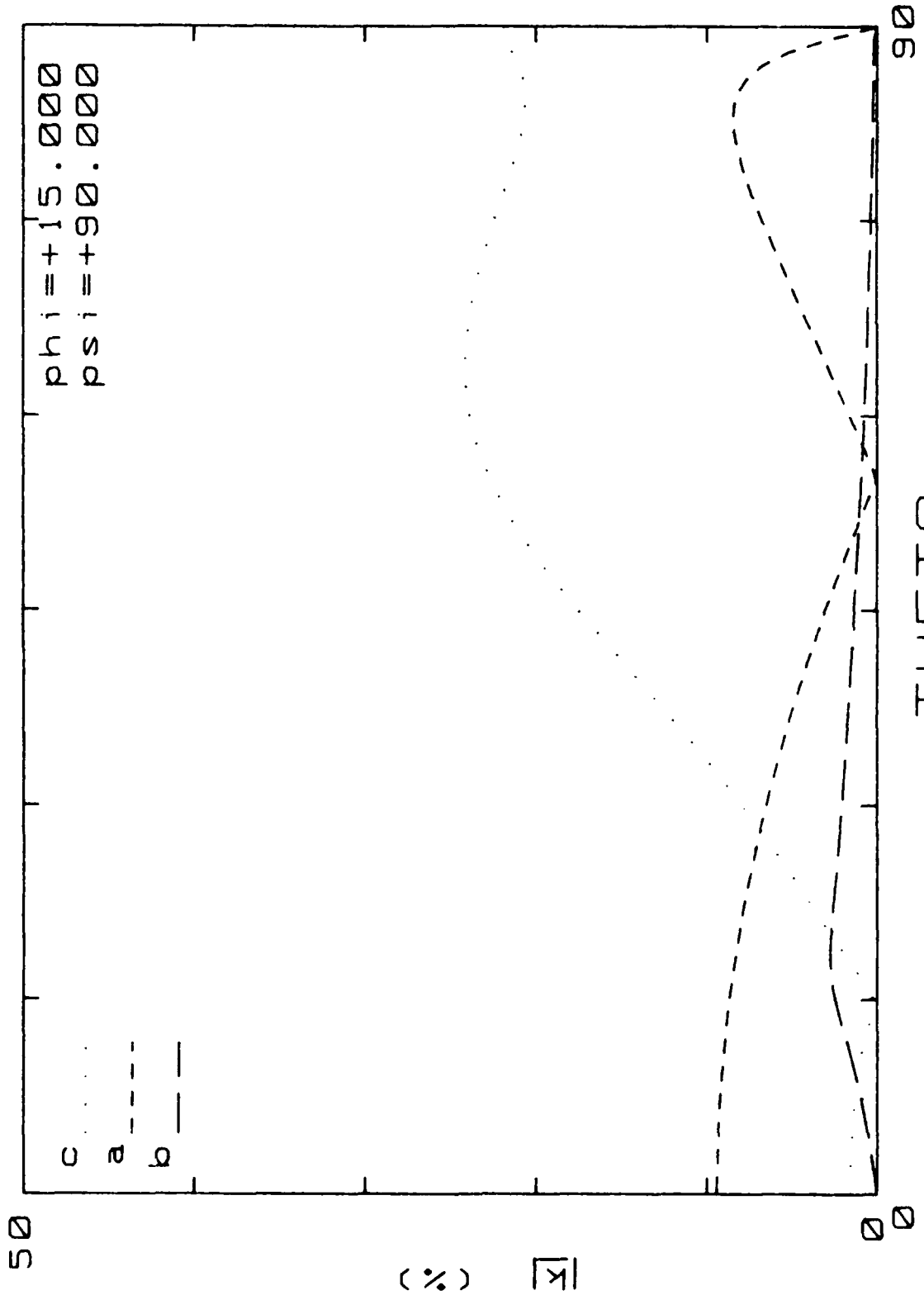


Figure 12. Piezocoupling, k_m, for (yxwl)ϕ=15°/θ, psi=90° cuts.

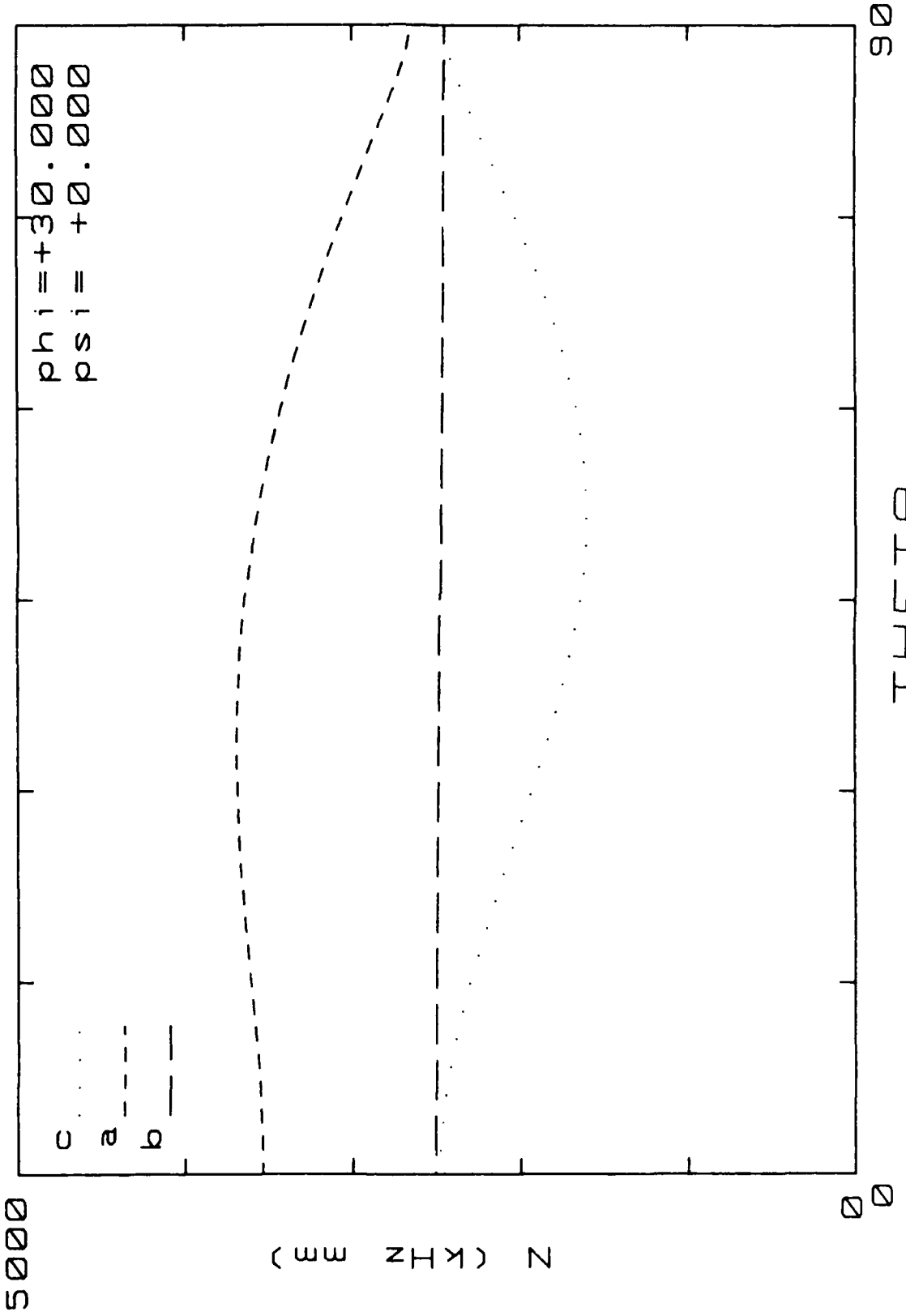


Figure 13. Frequency constant, N_m, for (yxwl)ϕ = 30°/θ cuts.

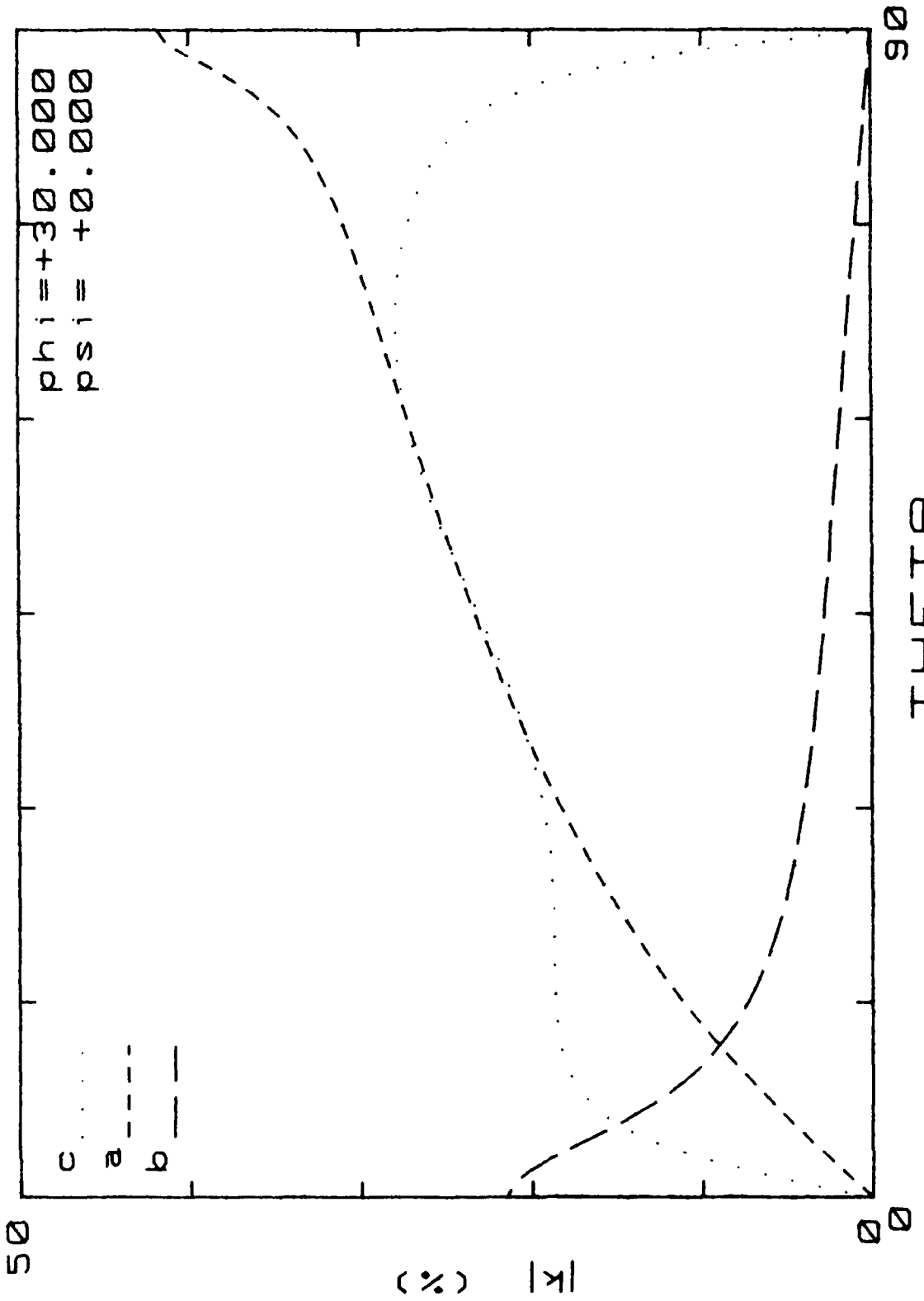


Figure 14. Piezocoupling, k_m, for (yxwl)ϕ=30°/θ cuts.

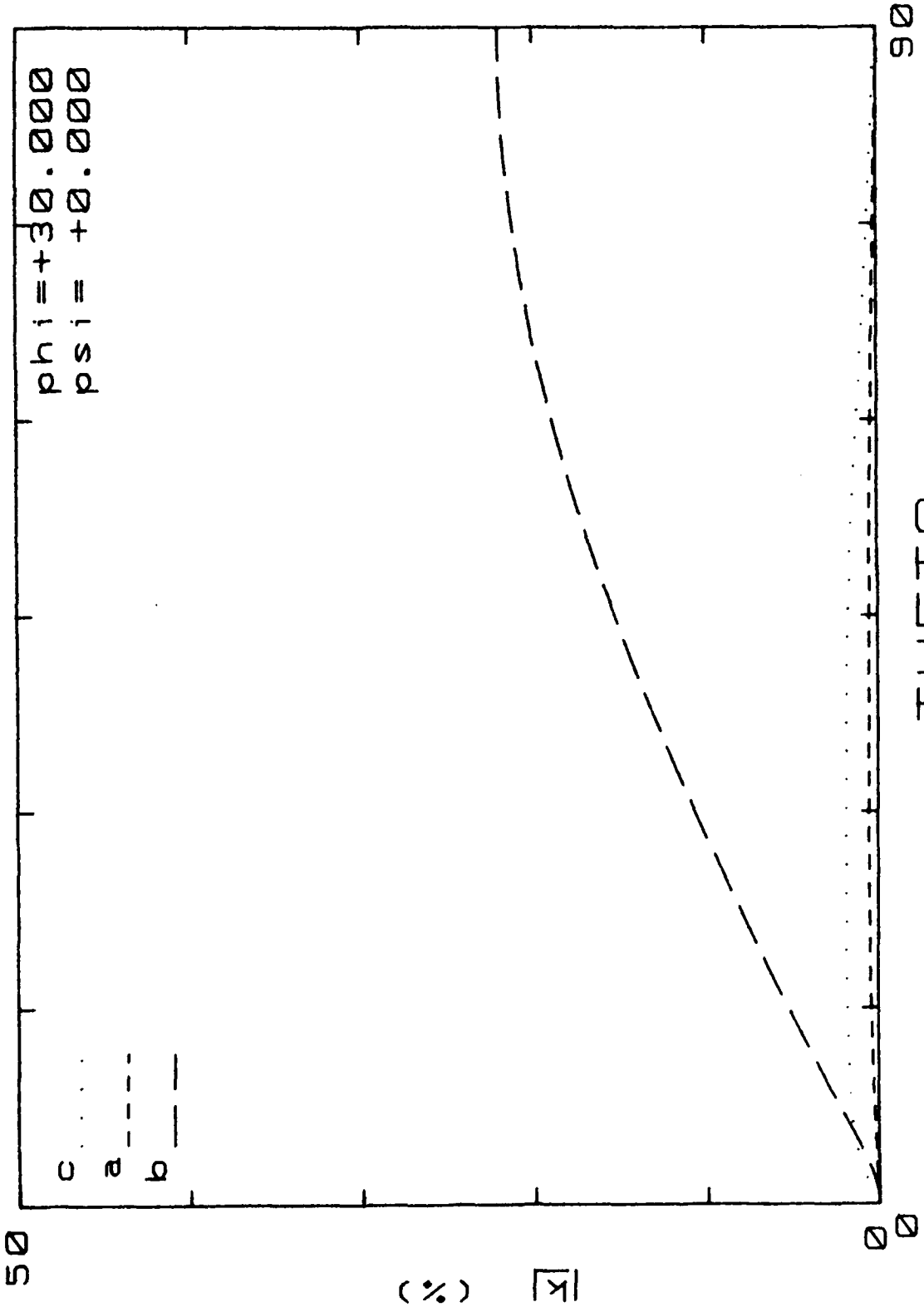


Figure 15. Piezocoupling, k_m, for (yxwl) ϕ=30°/θ, psi=0° cuts.

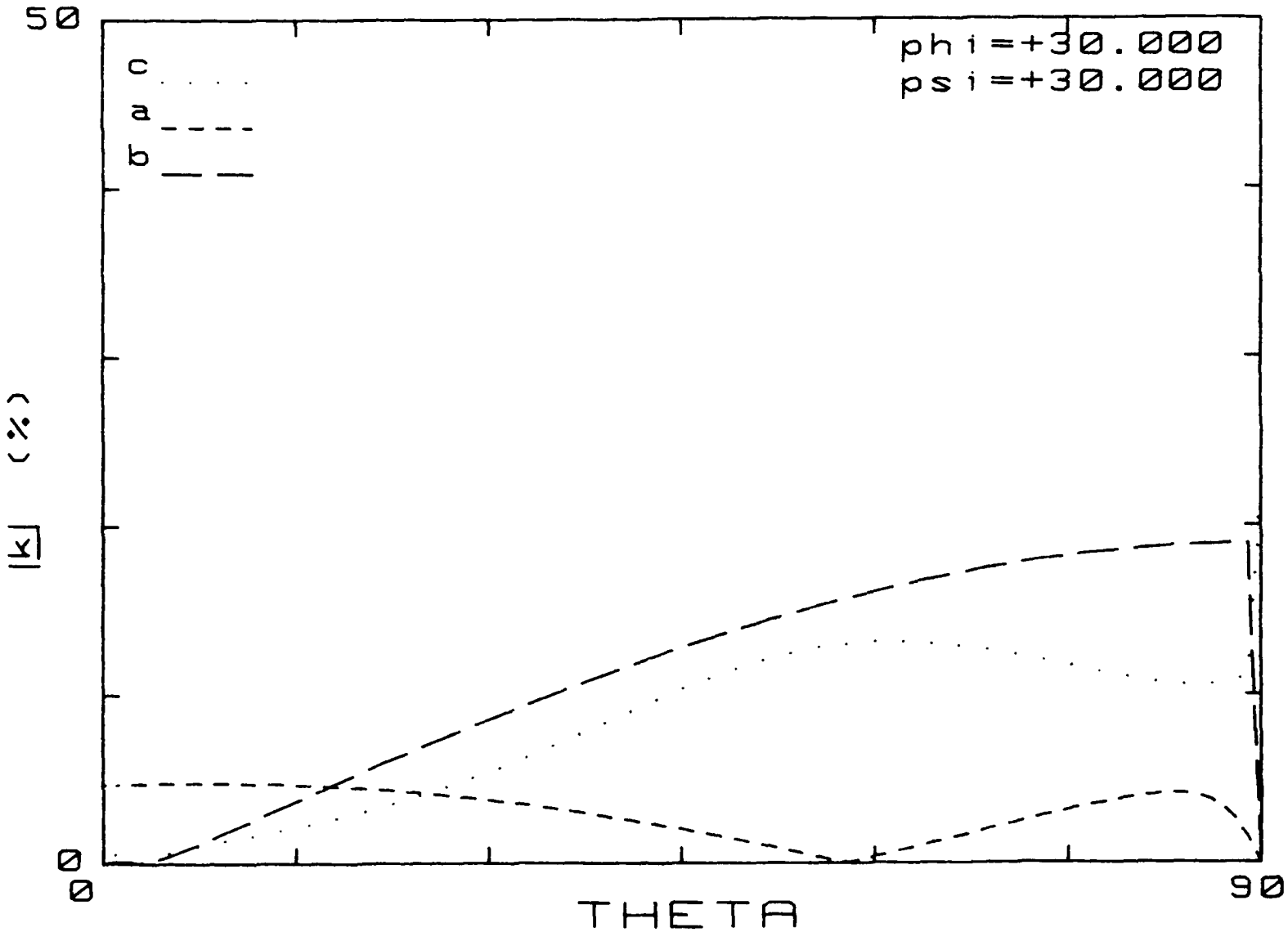


Figure 16. Piezocoupling, $\underline{k}_m$, for (yxwl)ϕ=30°/θ, psi=30° cuts.

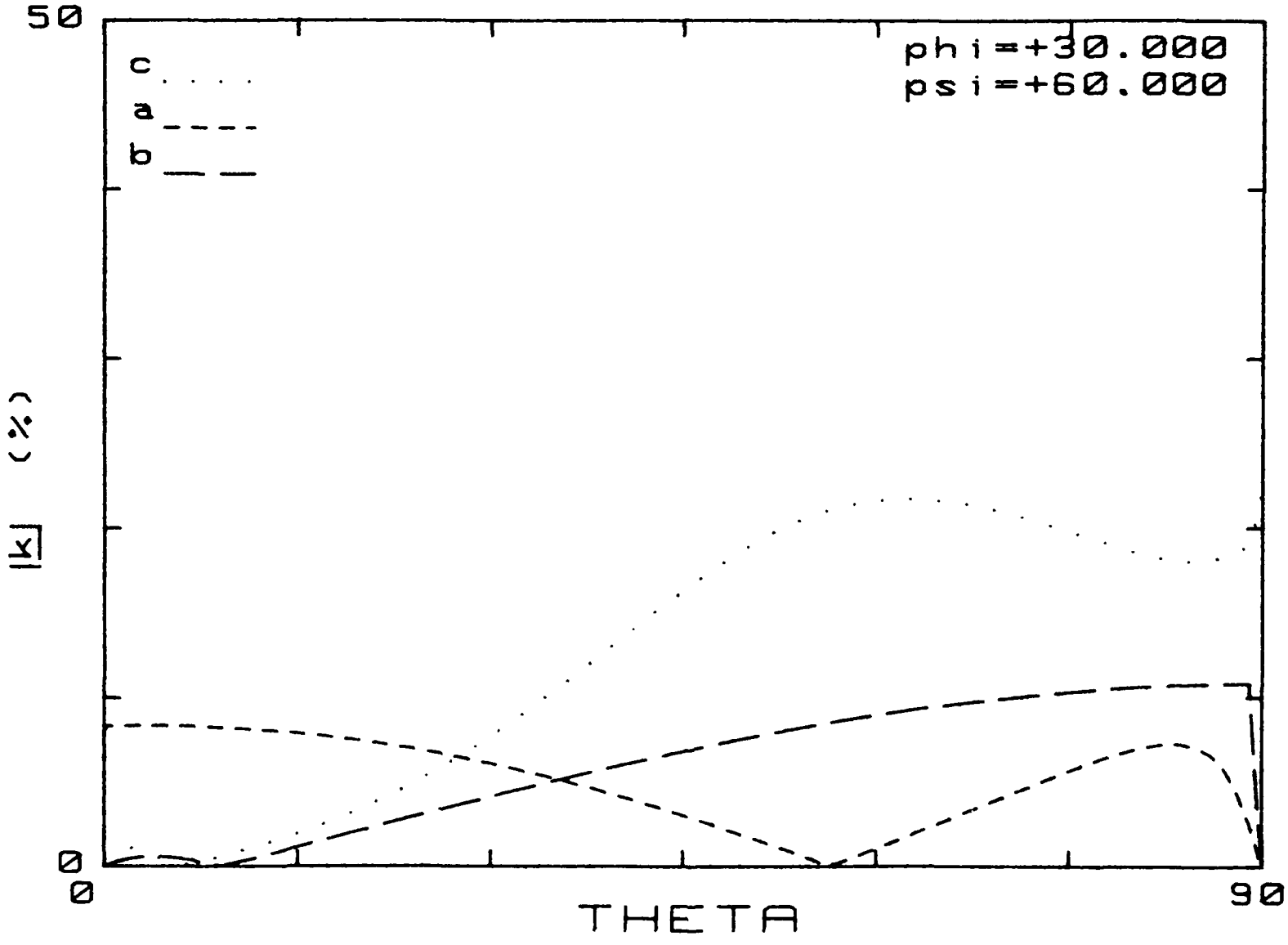


Figure 17. Piezocoupling, $\underline{k}_m$, for (yxwl)ϕ =30°/θ, psi=60° cuts.

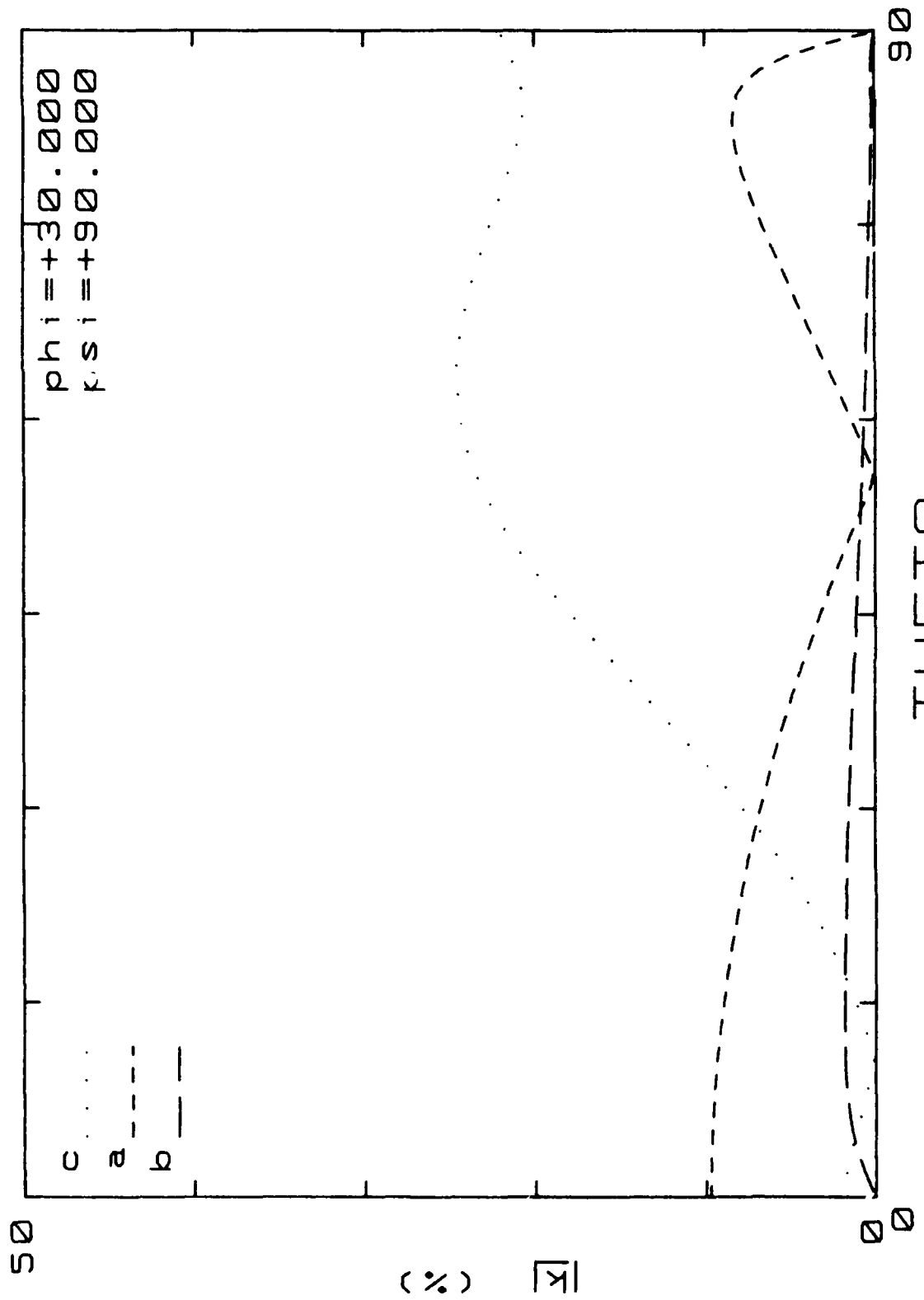


Figure 18. Piezocoupling, k_m, for (yxwl)ϕ :30°/θ, psi=90° cuts.

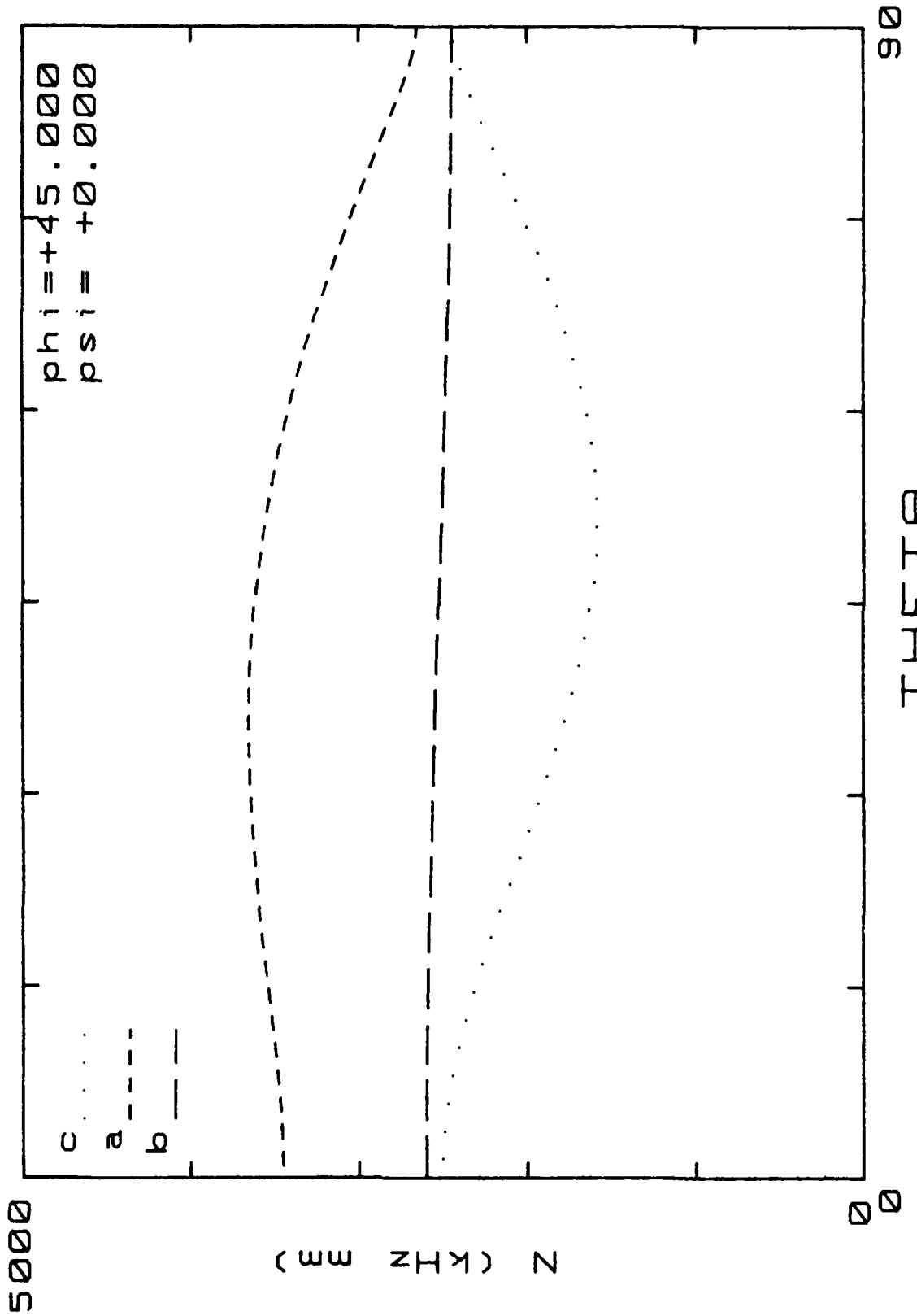


Figure 19. Frequency constant, N_m, for (yxwl)ϕ =45°/θcuts.

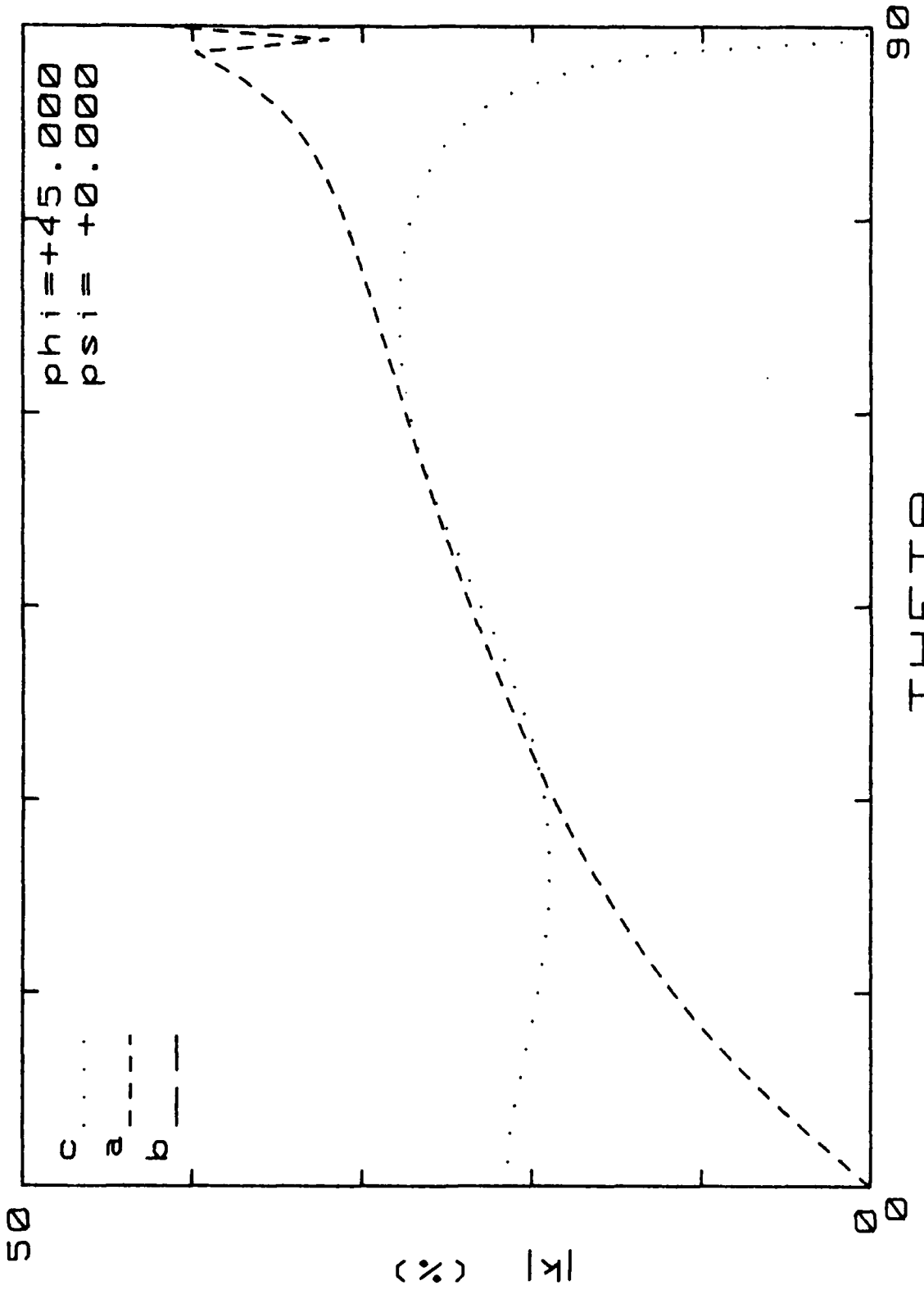


Figure 20. Piezocoupling, k_m, for (yxwl)ϕ =45°/θ cuts.

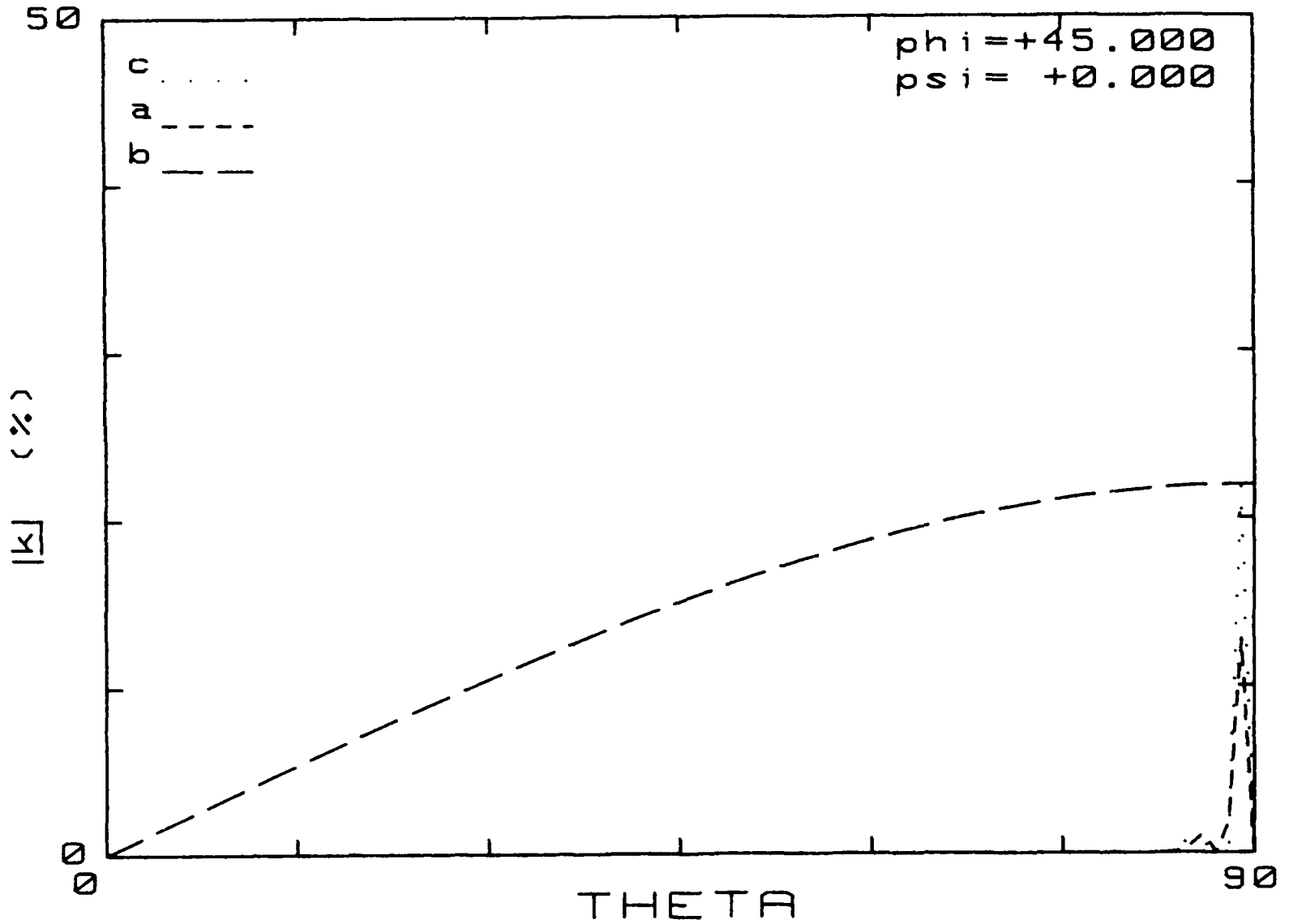


Figure 21. Piezocoupling, $\underline{k}_m$, for (yxwl)ϕ =45°/θ, psi=0° cuts.

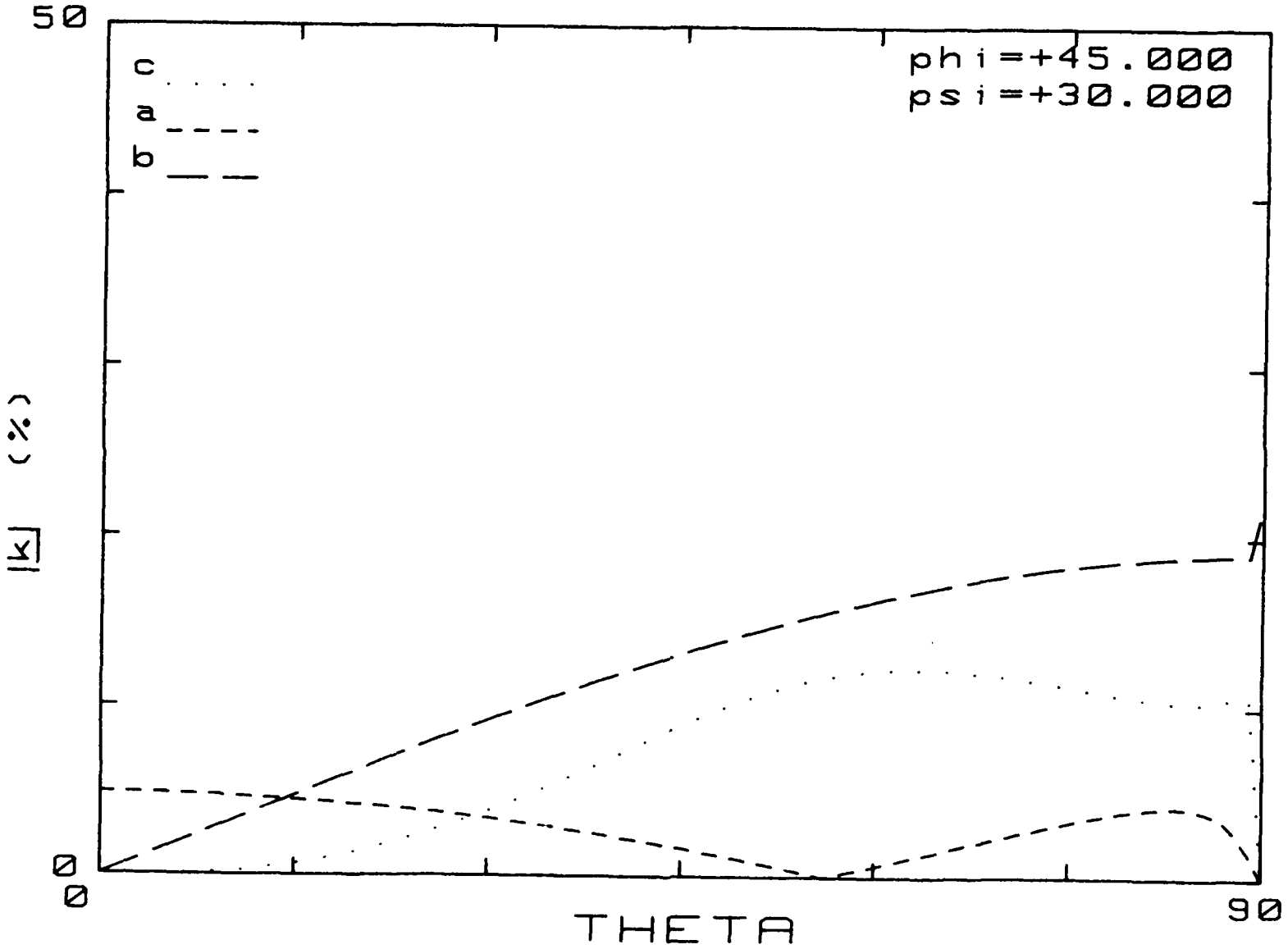


Figure 22. Piezocoupling, $\underline{k}_m$, for (yxwl)ϕ =45°/θ, psi=30° cuts.

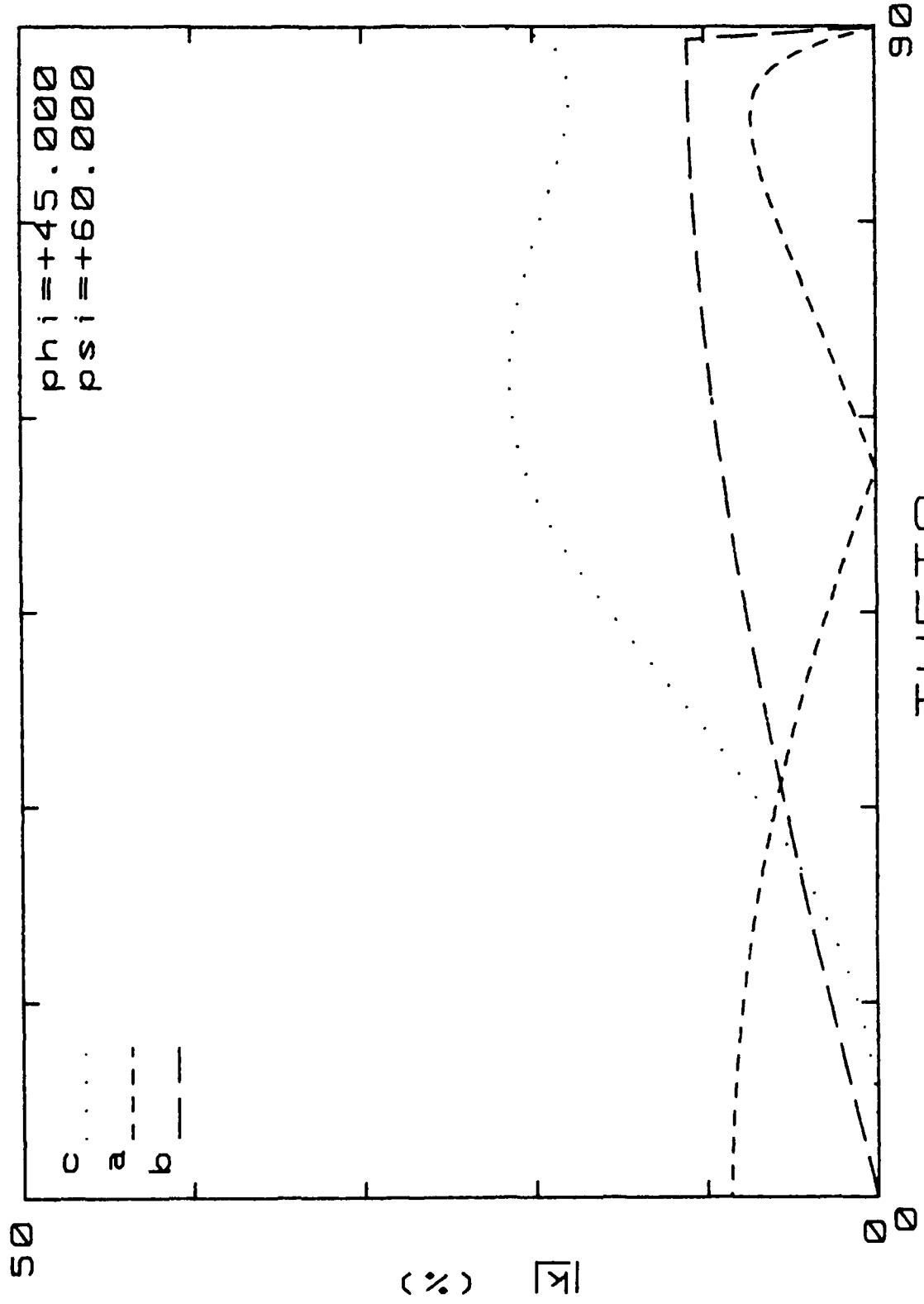


Figure 23. Piezocoupling, $k_{\overline{m}}$, for (yxwl)ϕ =45°/θ, psi=60° cuts.

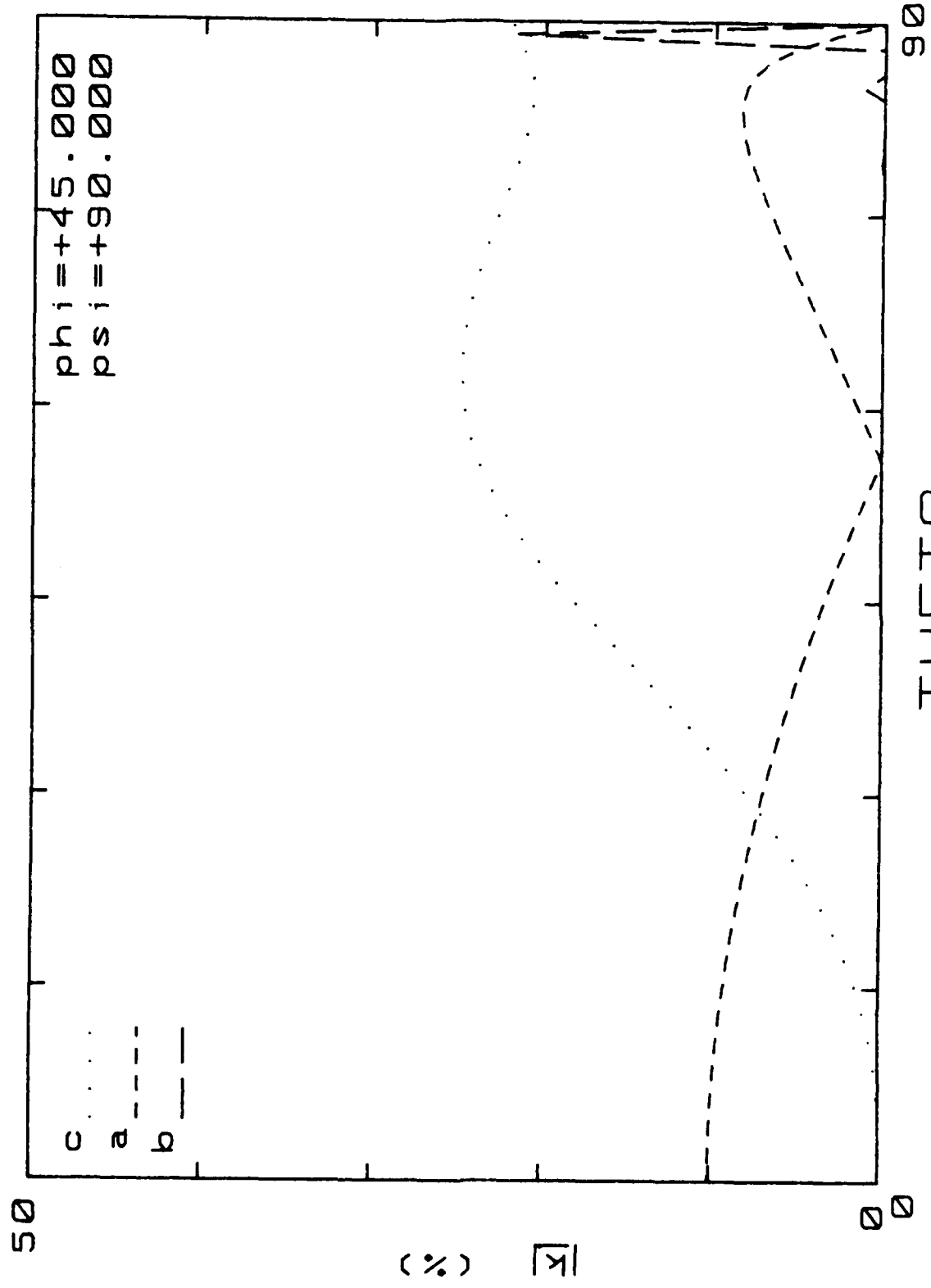


Figure 24. Piezocoupling, k_m, for (yxwl)ϕ =45°/θ, psi=90° cuts.

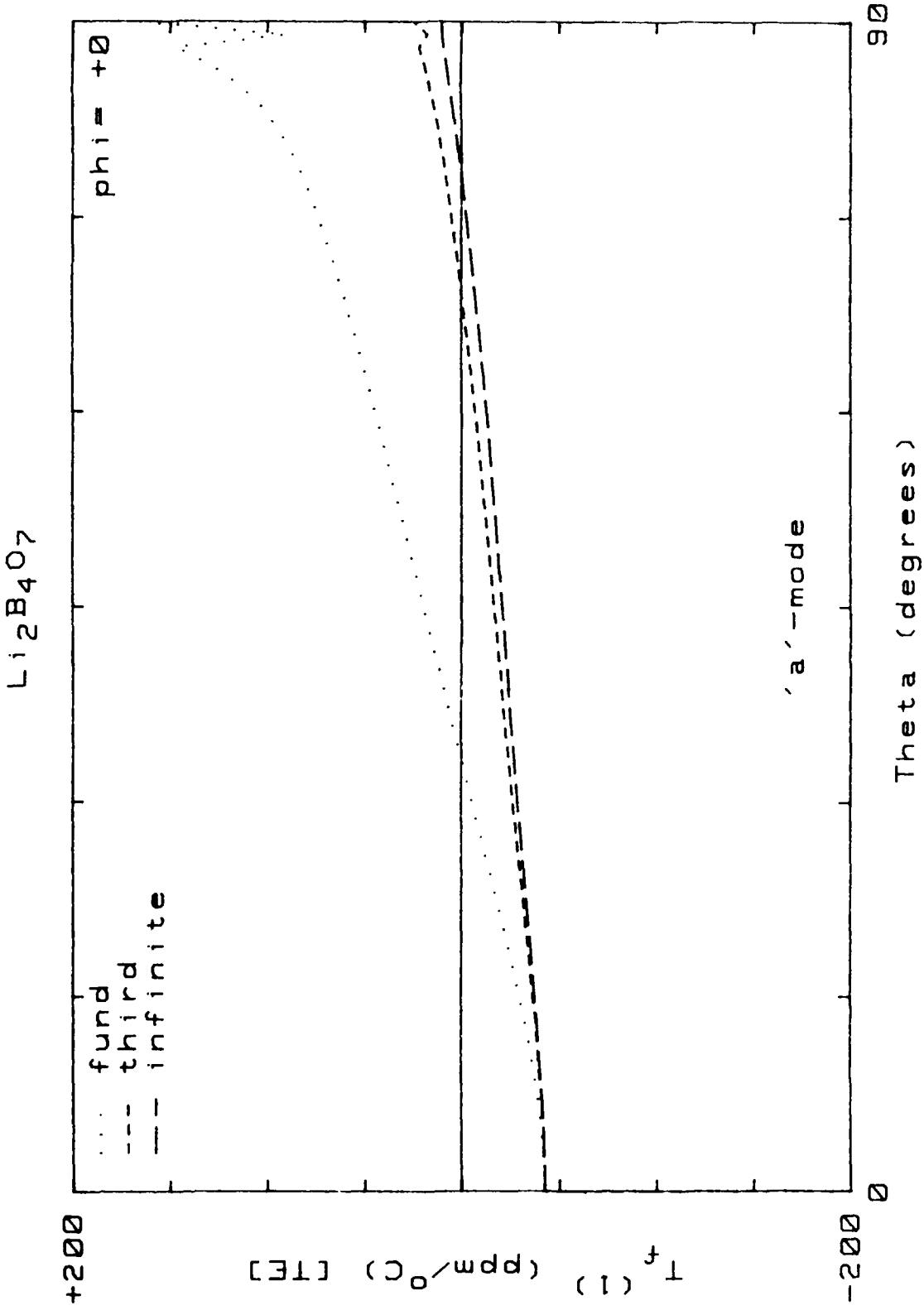


Figure 25. TC(1) for (yxwl)ϕ=0°/θ cuts; N = 1, 3,∞; mode "a"; [TE].

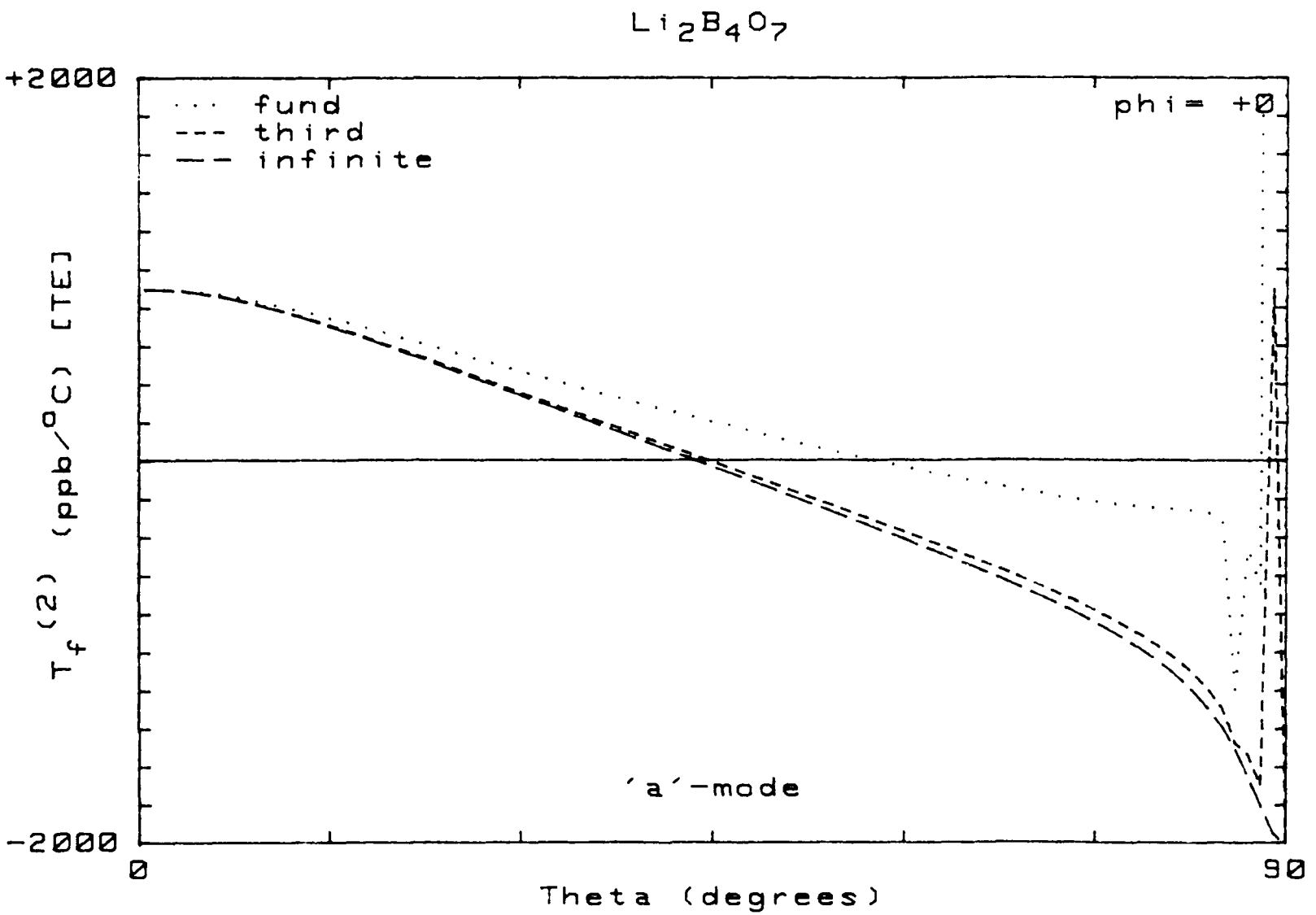


Figure 26. TC(2) for (yxwl)ϕ =0°/θ cuts; M = 1, 3,∞ ; mode "a"; [TE].

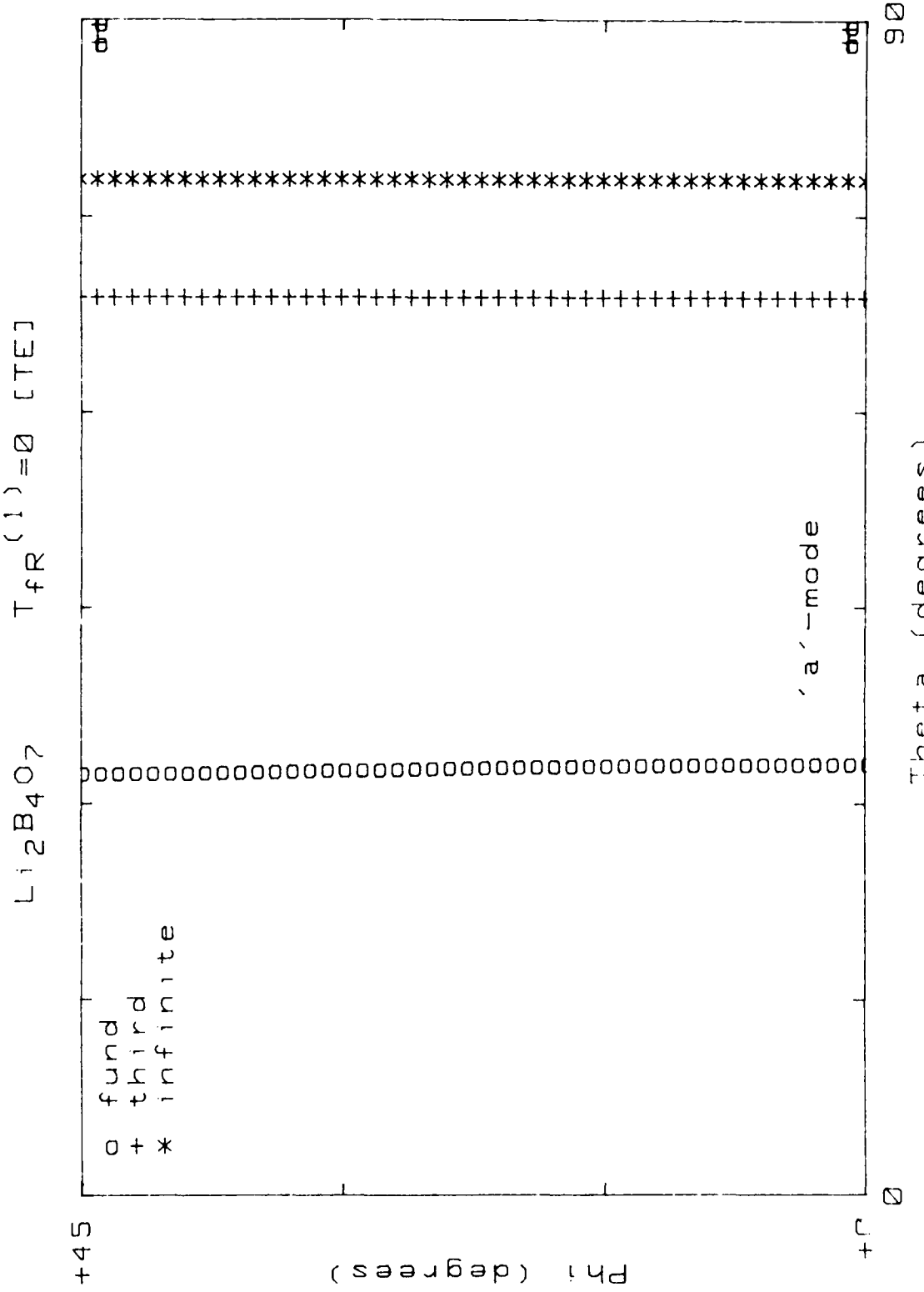
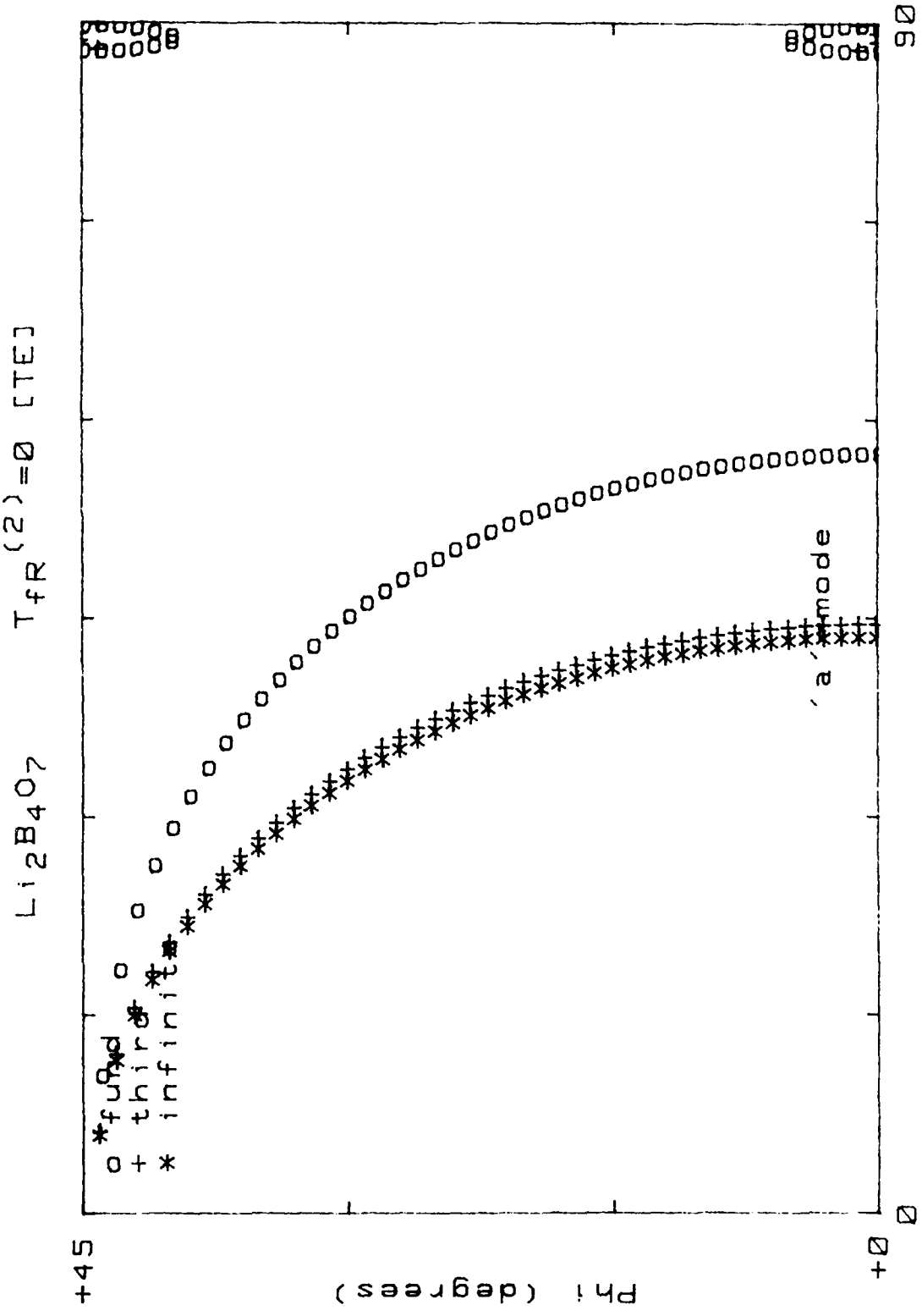


Figure 27. Locus of TC(1)=0 for (yxwl)ϕ/θcuts; M = 1, 3,∞ ; mode "a"; [TE].



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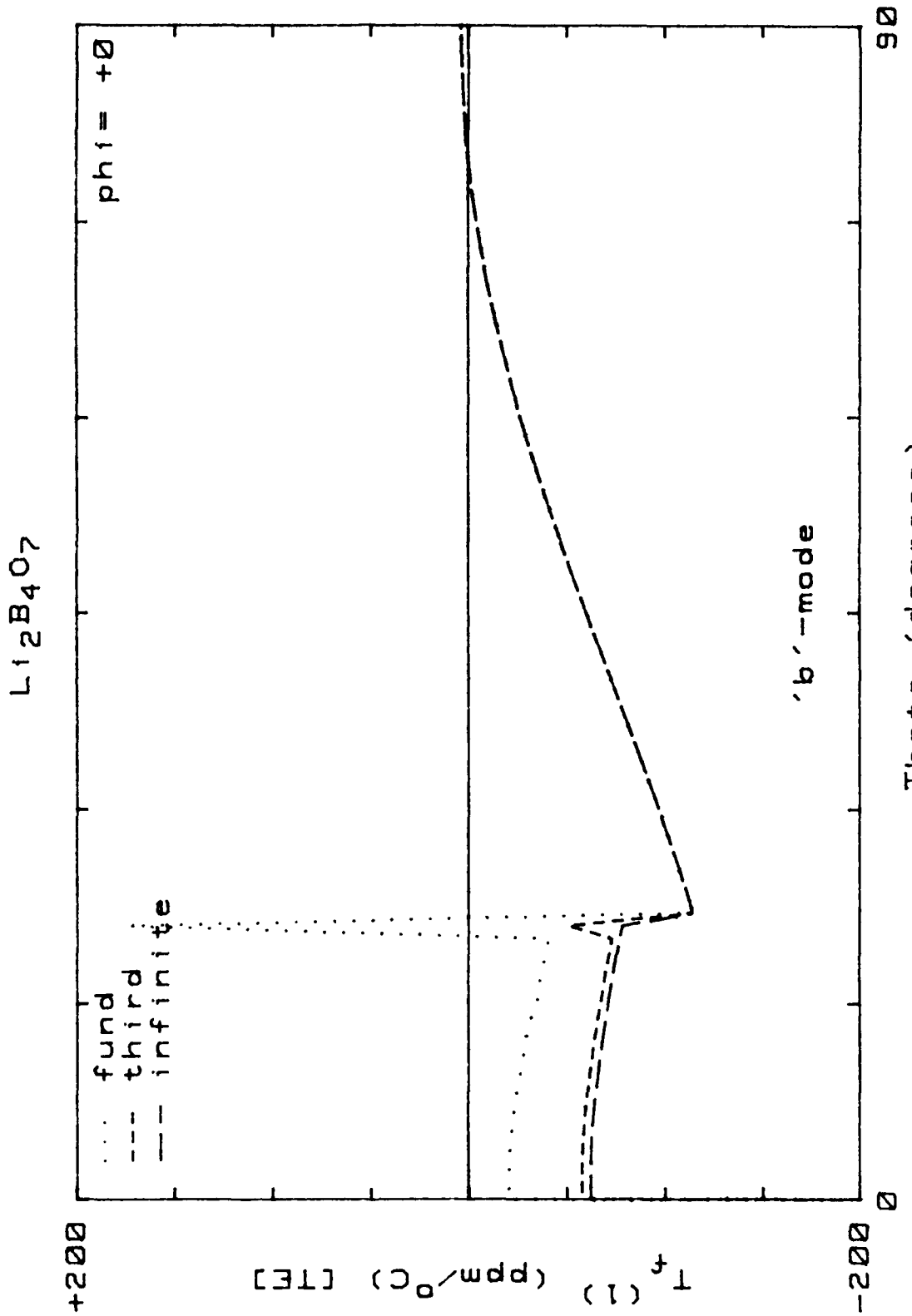

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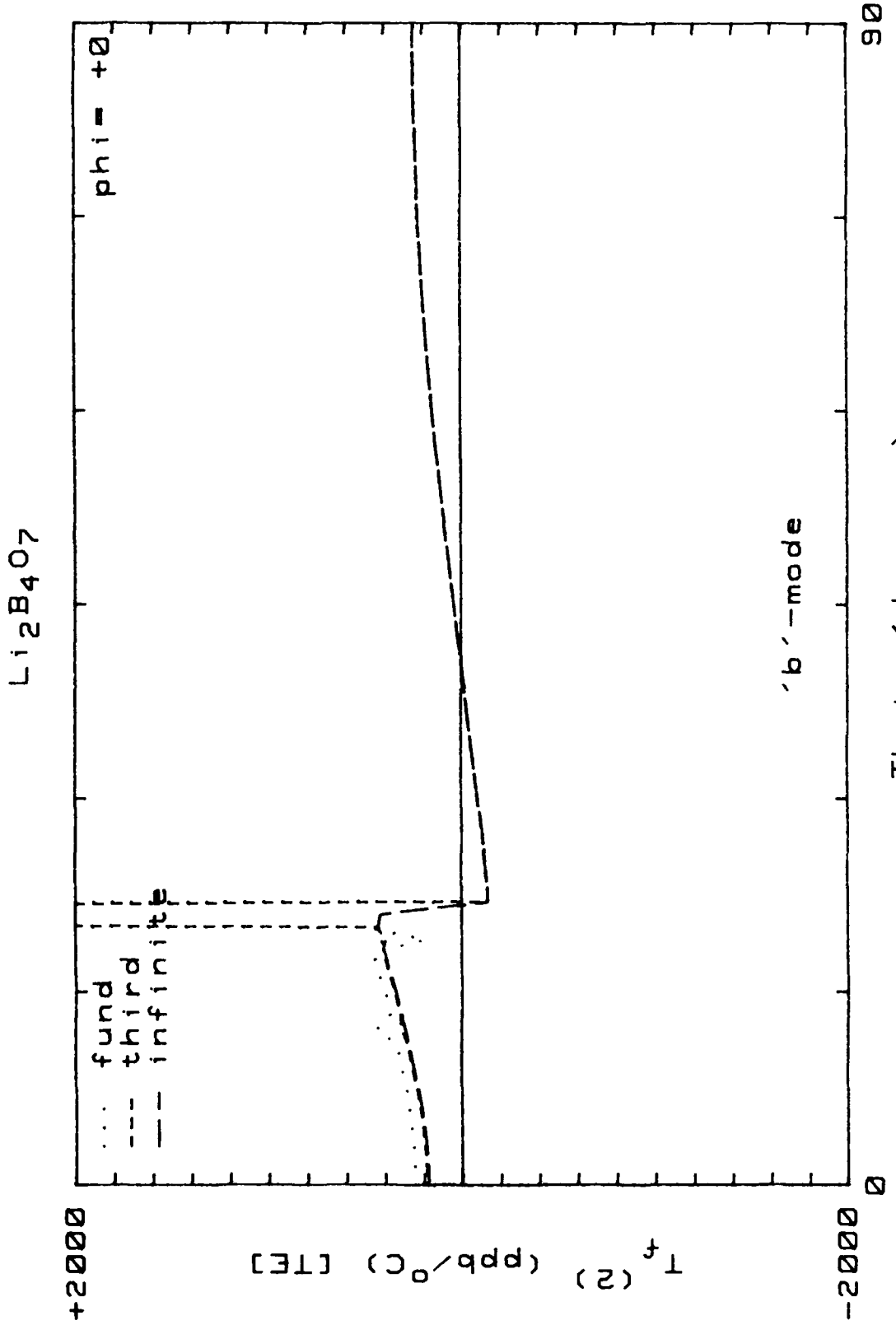

Figure 30. TC(2) for (yxwl)ϕ=0°/θ cuts; M = 1, 3,∞; mode "b"; [TE].

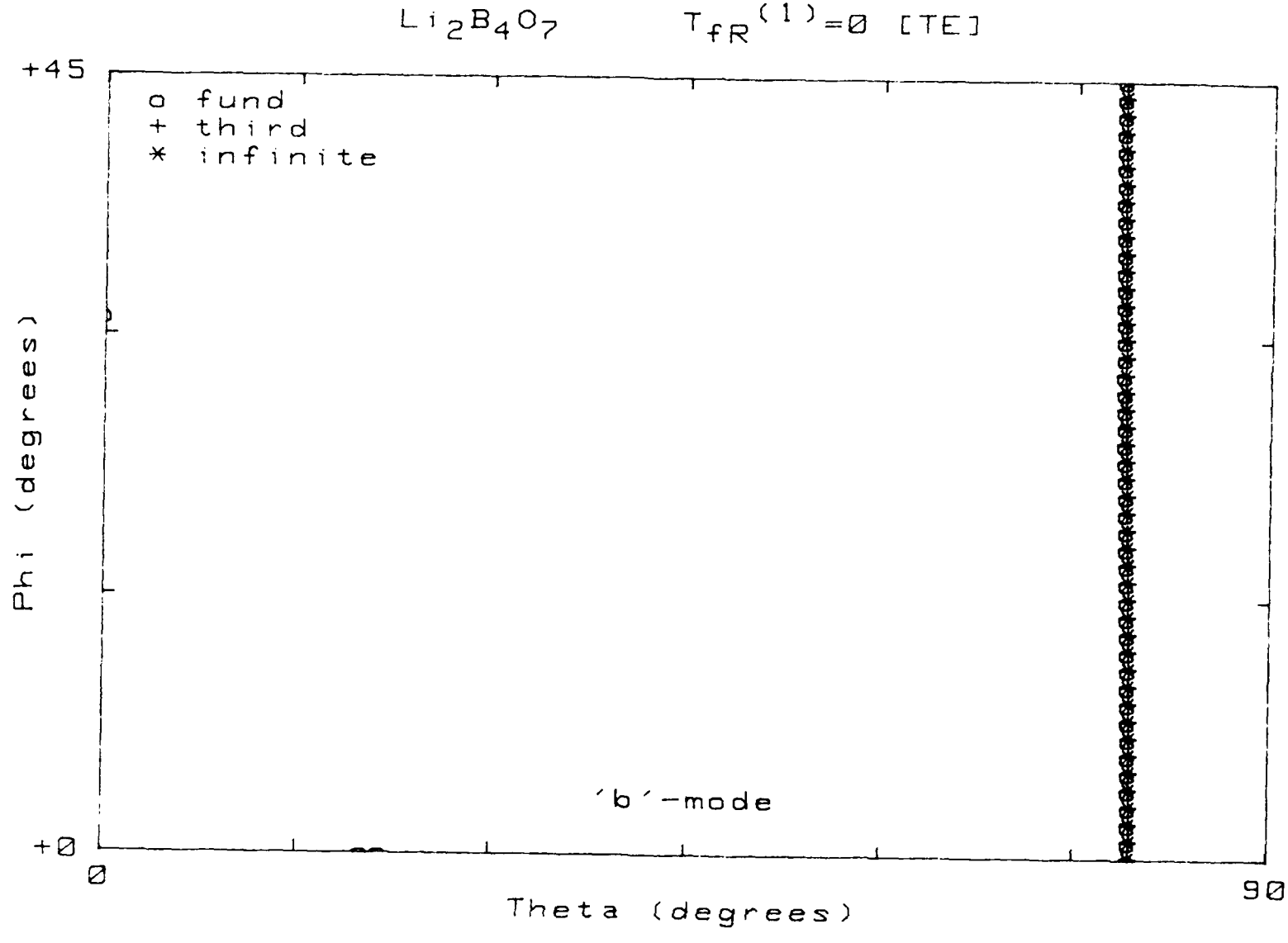

Figure 31. Locus of TC(1)=0 for (yxwl)ϕ/θ cuts; M = 1, 3, ∞; mode "b"; [TE].

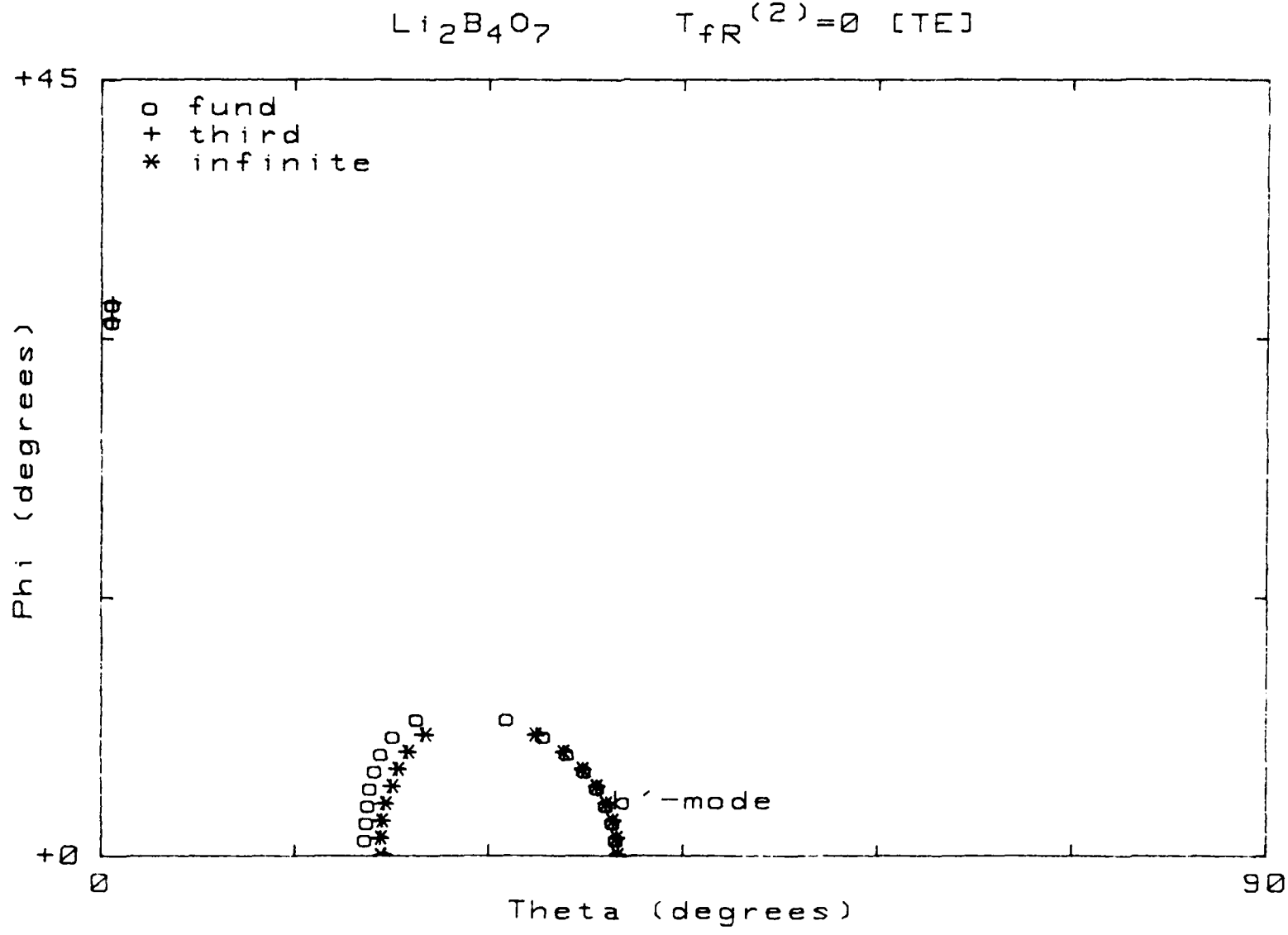

Figure 32. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M = 1, 3,∞ ; mode "b"; [TE].

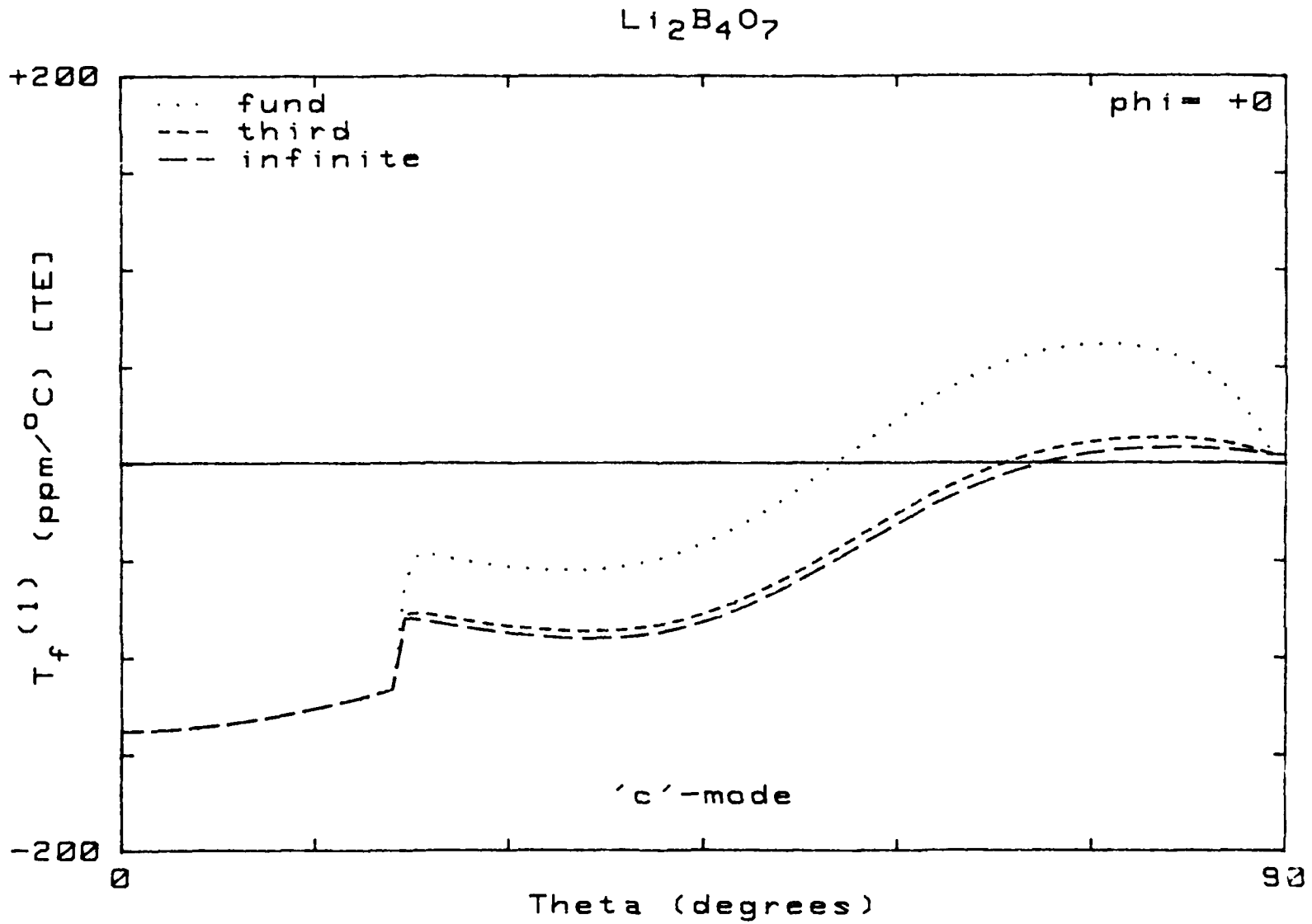

Figure 33. TC(1) for (yxwl)ϕ=0°/θ cuts; M = 1, 3, ∞; mode "c"; [TE].

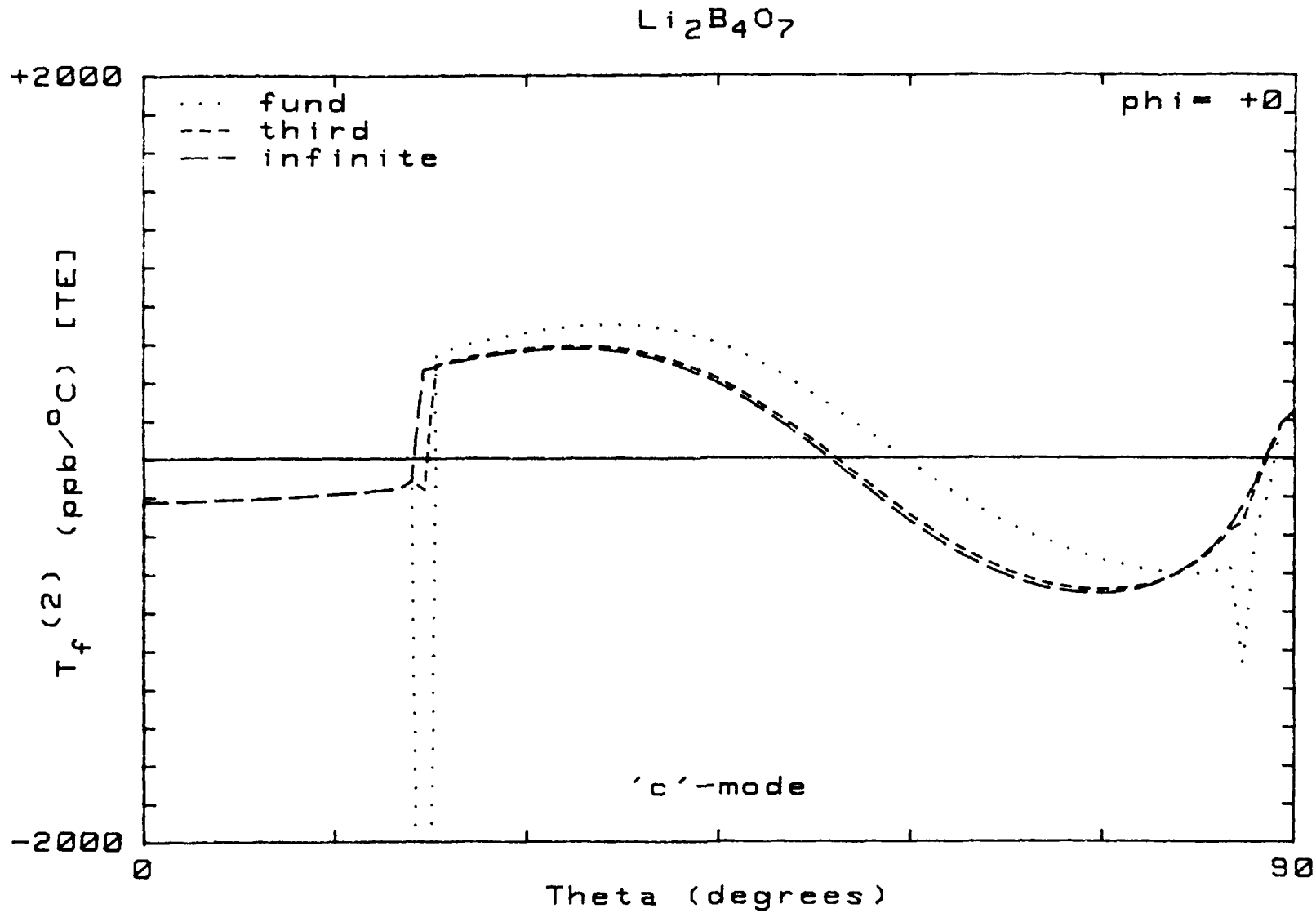

Figure 34. TC(2) for (yxwl)ϕ=0°/θ cuts; M = 1, 3,∞; mode "c"; [TE].

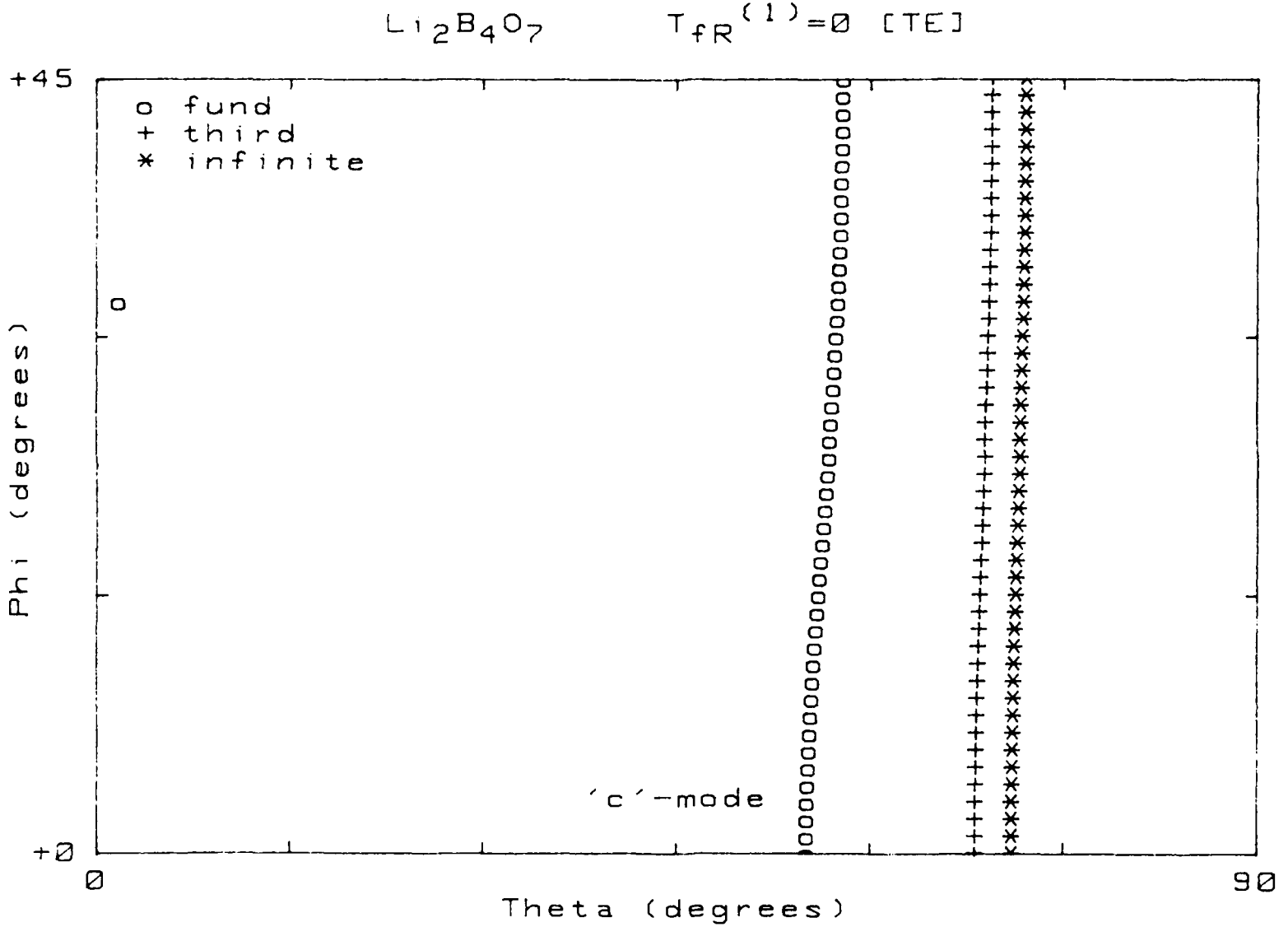

Figure 35. Locus of TC(1)=0 for (yxwl)ϕ/θ cuts; M = 1, 3,∞ ; mode "c"; [TE].

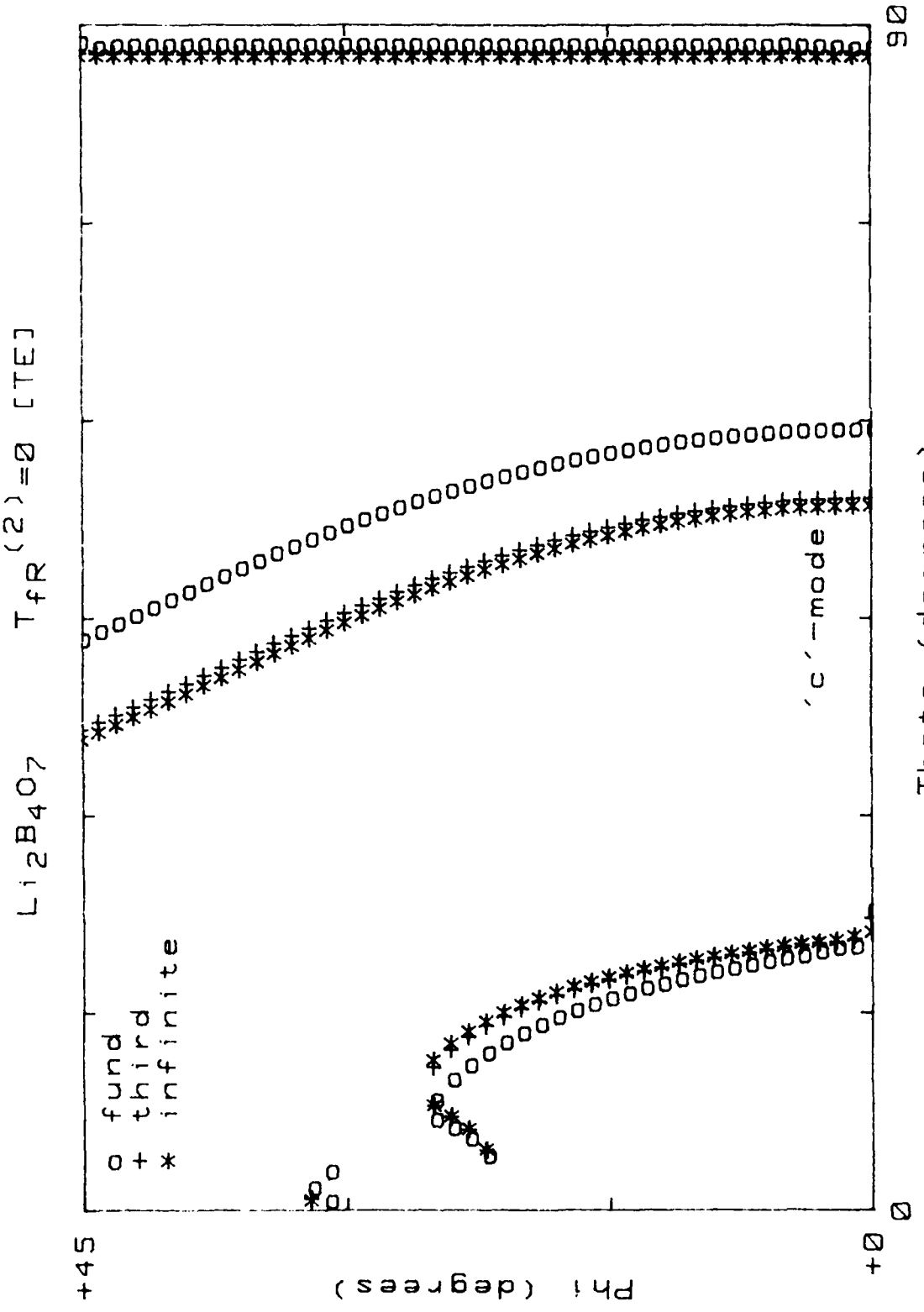

Figure 36. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M = 1, 3,∞ ; mode "c"; [TE].

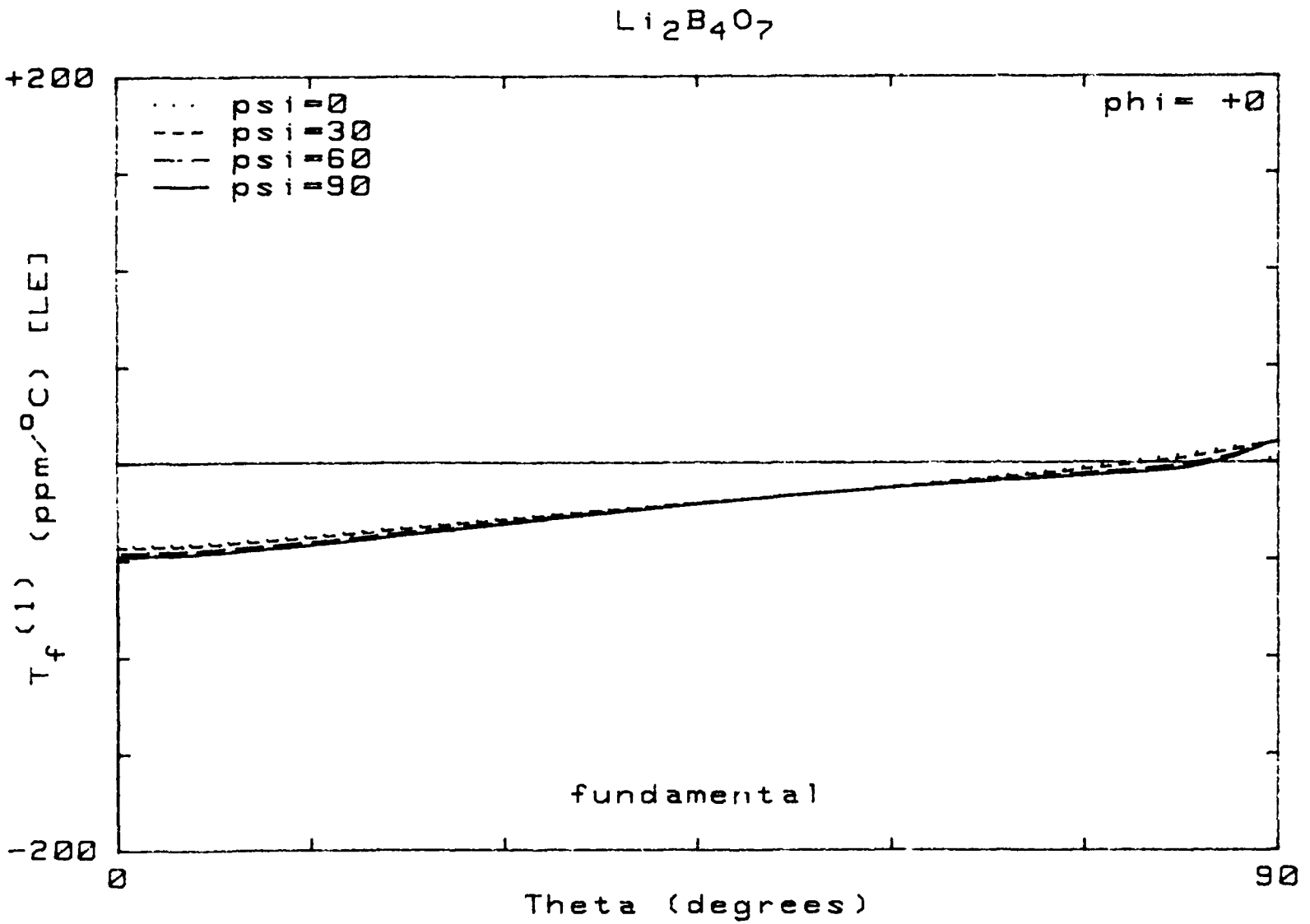

Figure 37. TC(1) for (yxwl)ϕ=0°/θ cuts; M = 1; mode "a"; psi=0°(30°)90°; [LE].

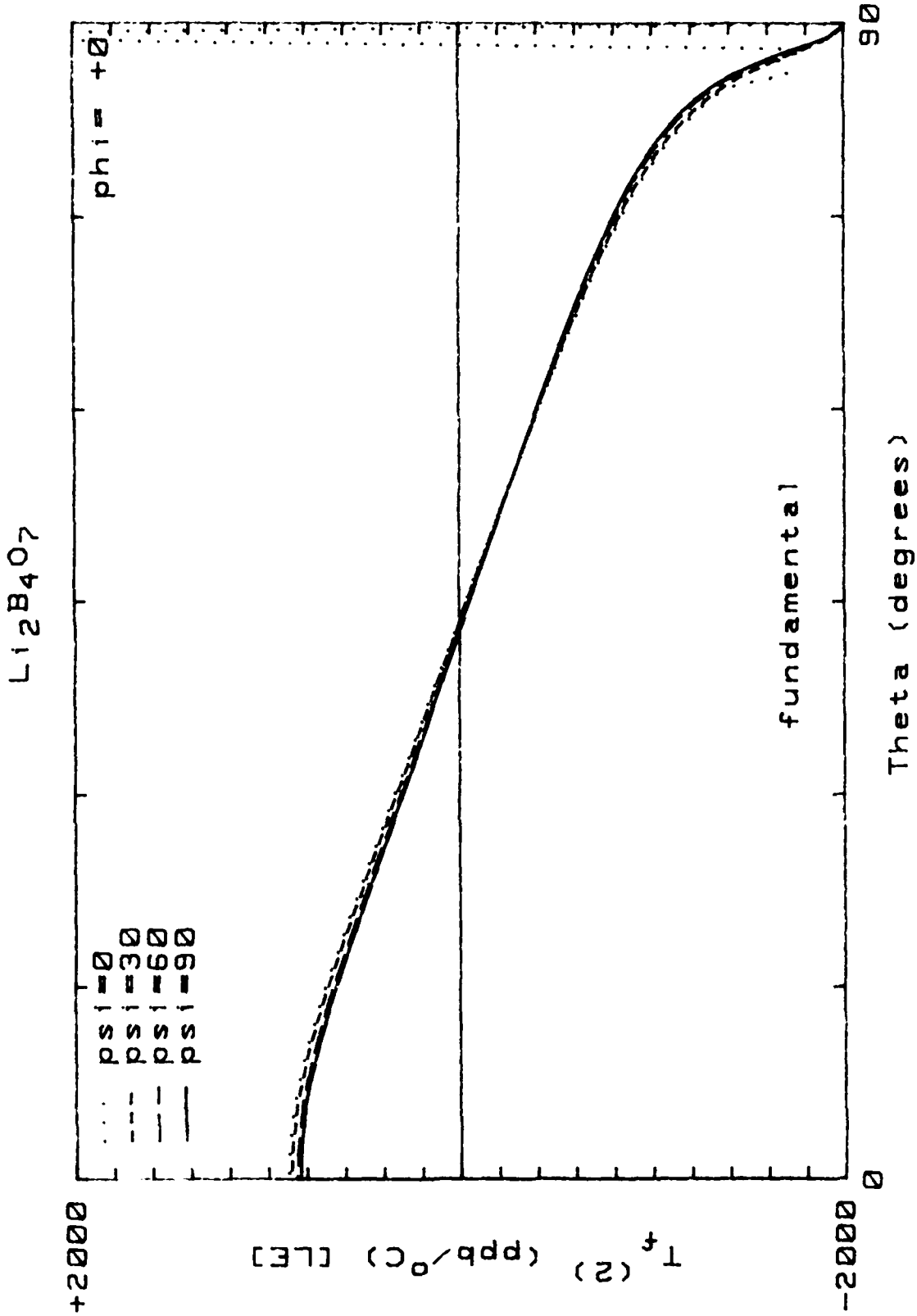

Figure 38. TC(2) for (yxwl) ϕ=0°/θ cuts; M = 1; mode "a"; psi=0° (30°)90°; [LE]

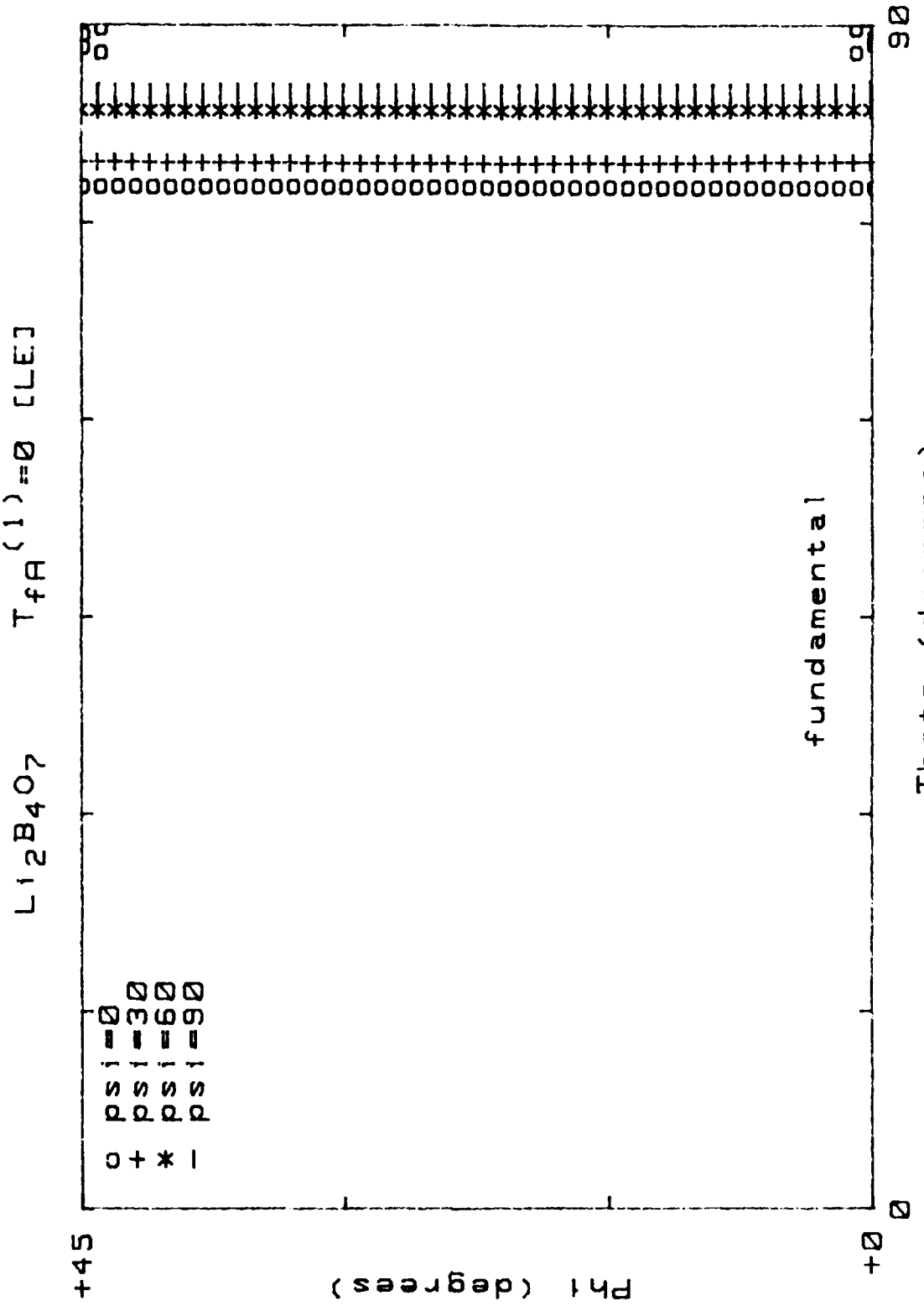

Figure 31. Locus of TC(1)=0 for (yxwl)ϕ/θ cuts; M = 1; mode "a"; psi=0° (30°)90°; [LE]

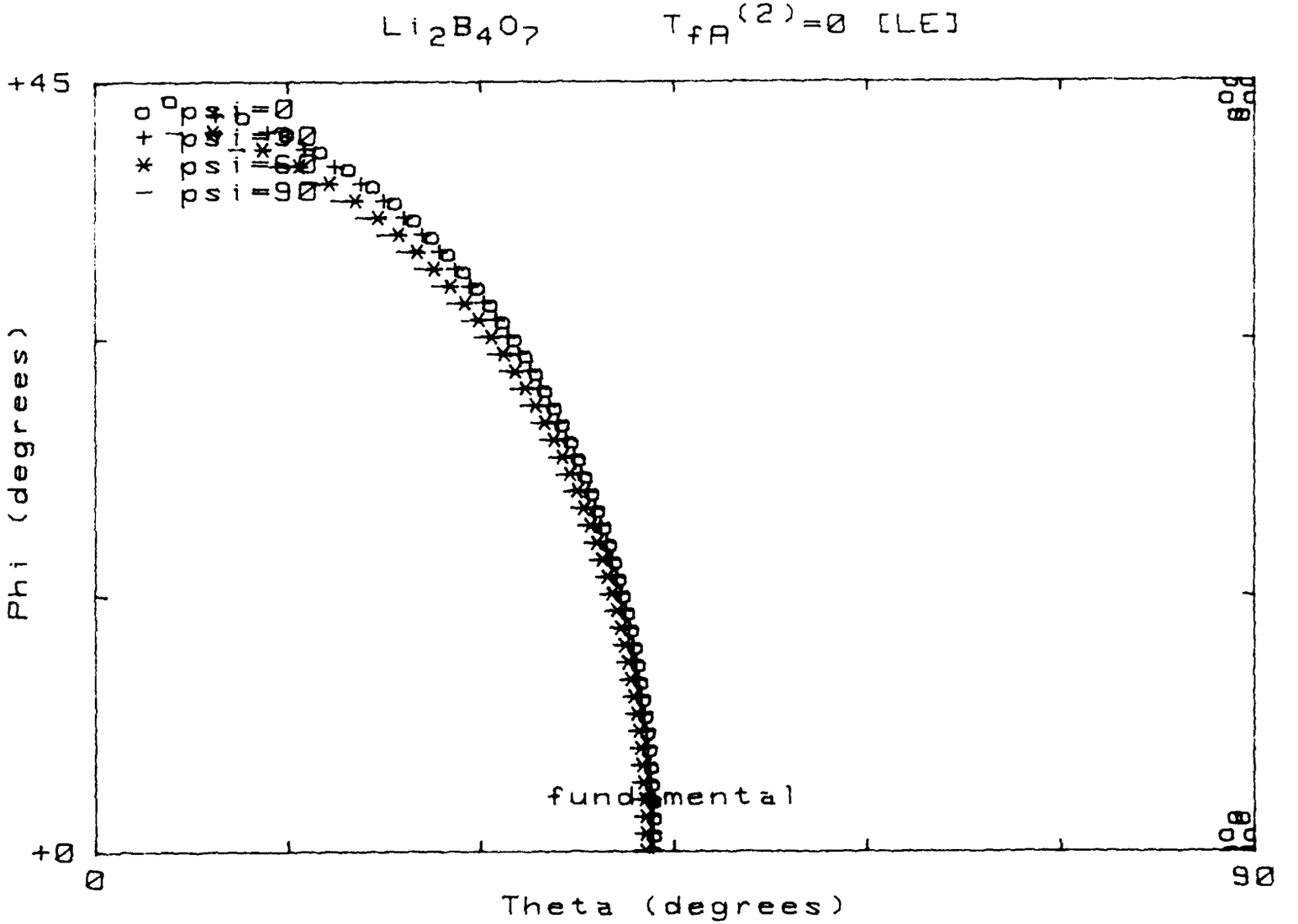

Figure 40. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M = 1; mode "a"; psi=0° (30°)90°; [LE]

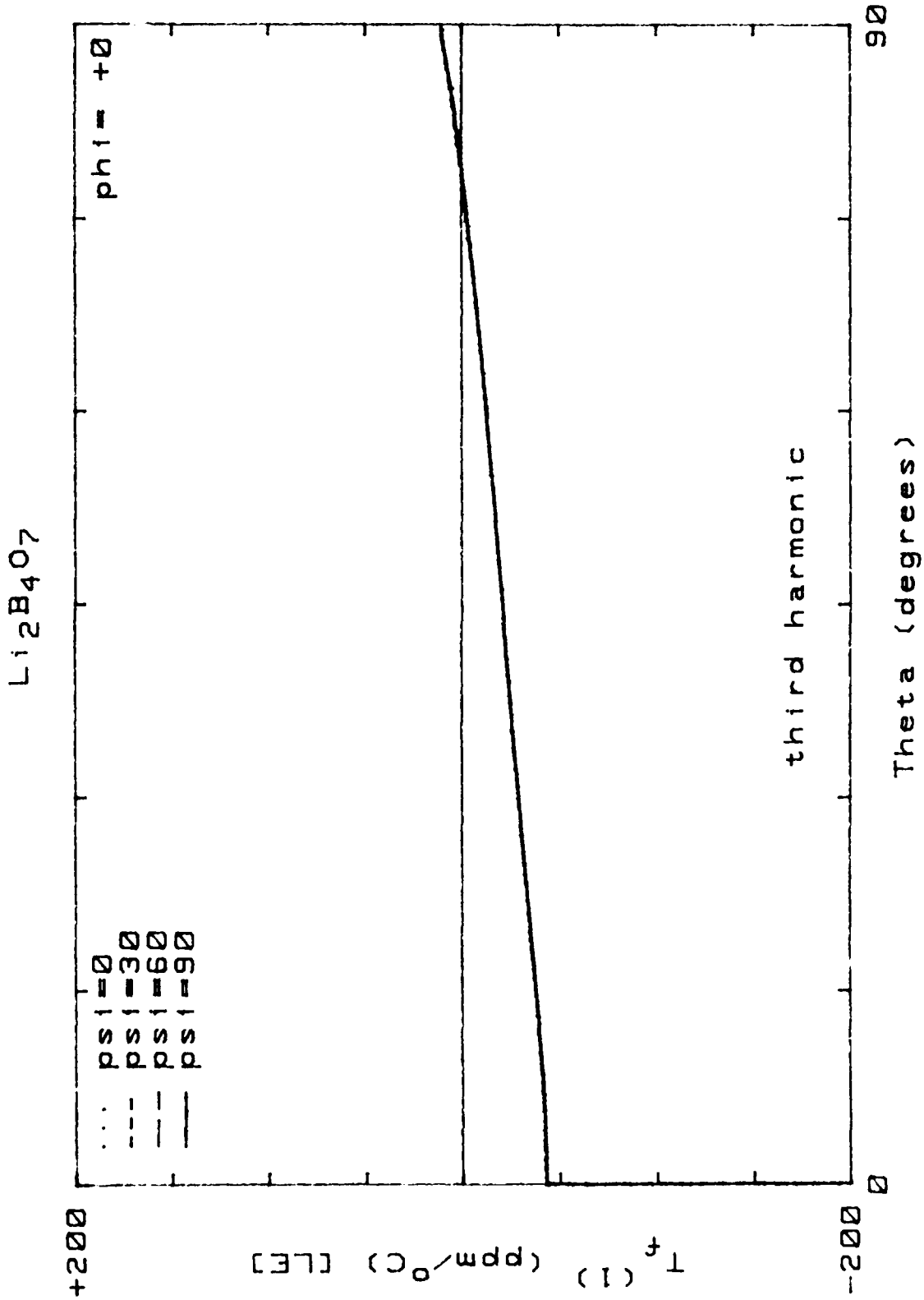

Figure 41. TC(1) for (yxwl)ϕ=0°/θ cuts; M = 3; mode "a"; psi=0° (30°)90°; [LE]

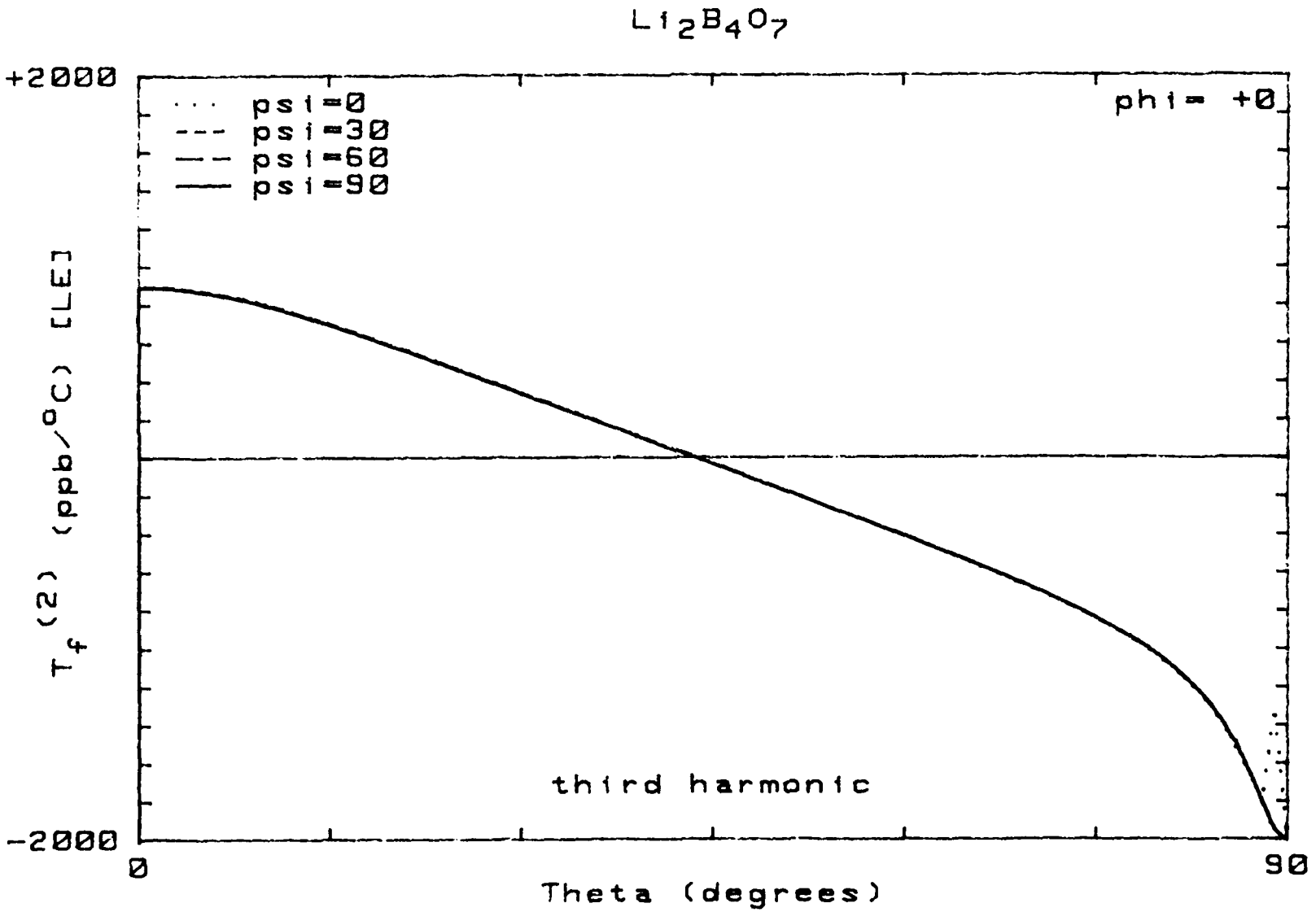

Figure 42. TC(2) for (yxwl)ϕ=0°/θ cuts; M = 3; mode "a"; psi=0° (30°)90°; [LE]

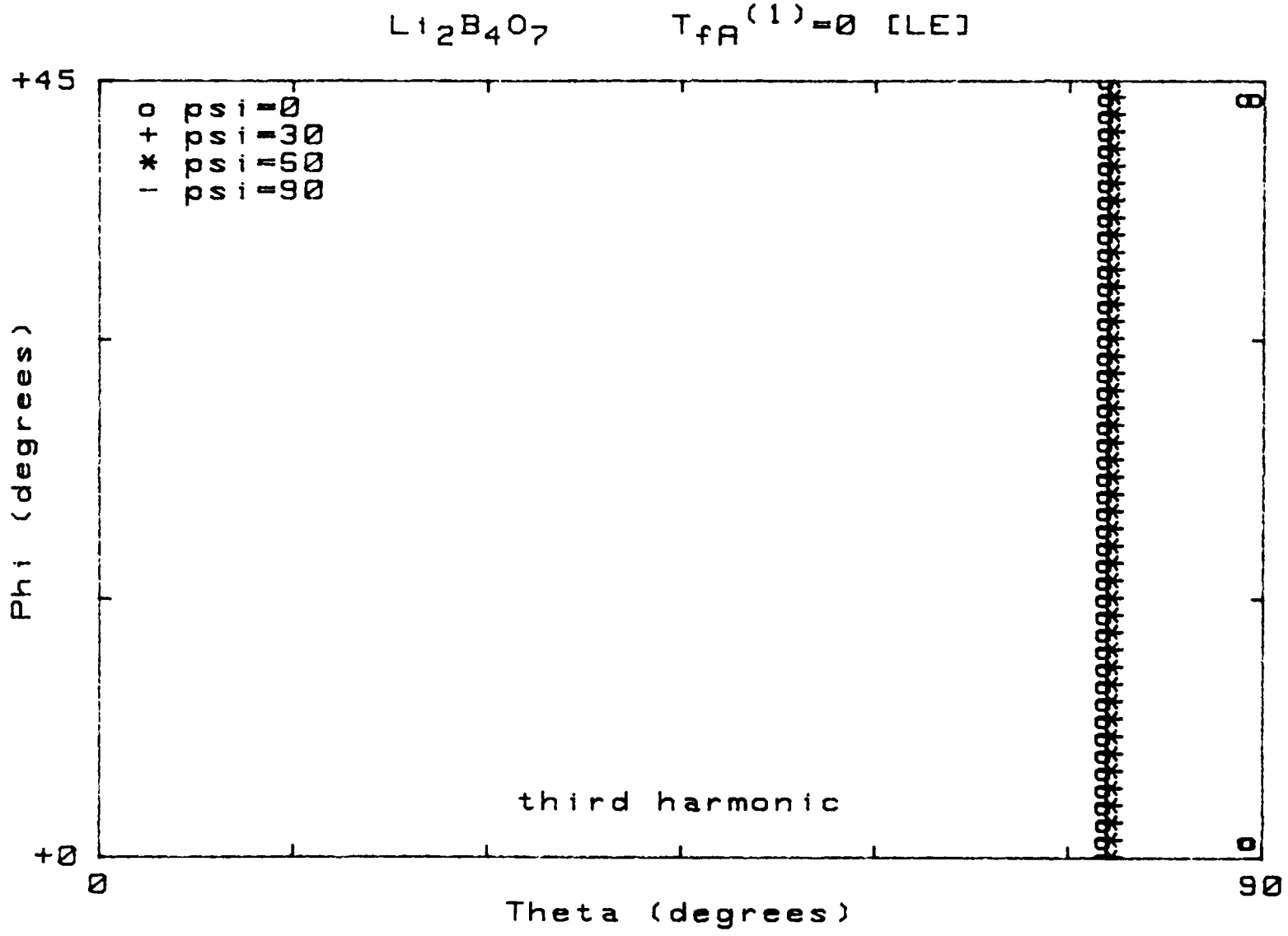

Figure 43. Locus of TC(1)=0 for (yxwl)ϕ/θ cuts; M = 3; mode "a"; psi=0° (30°)90°; [LE]

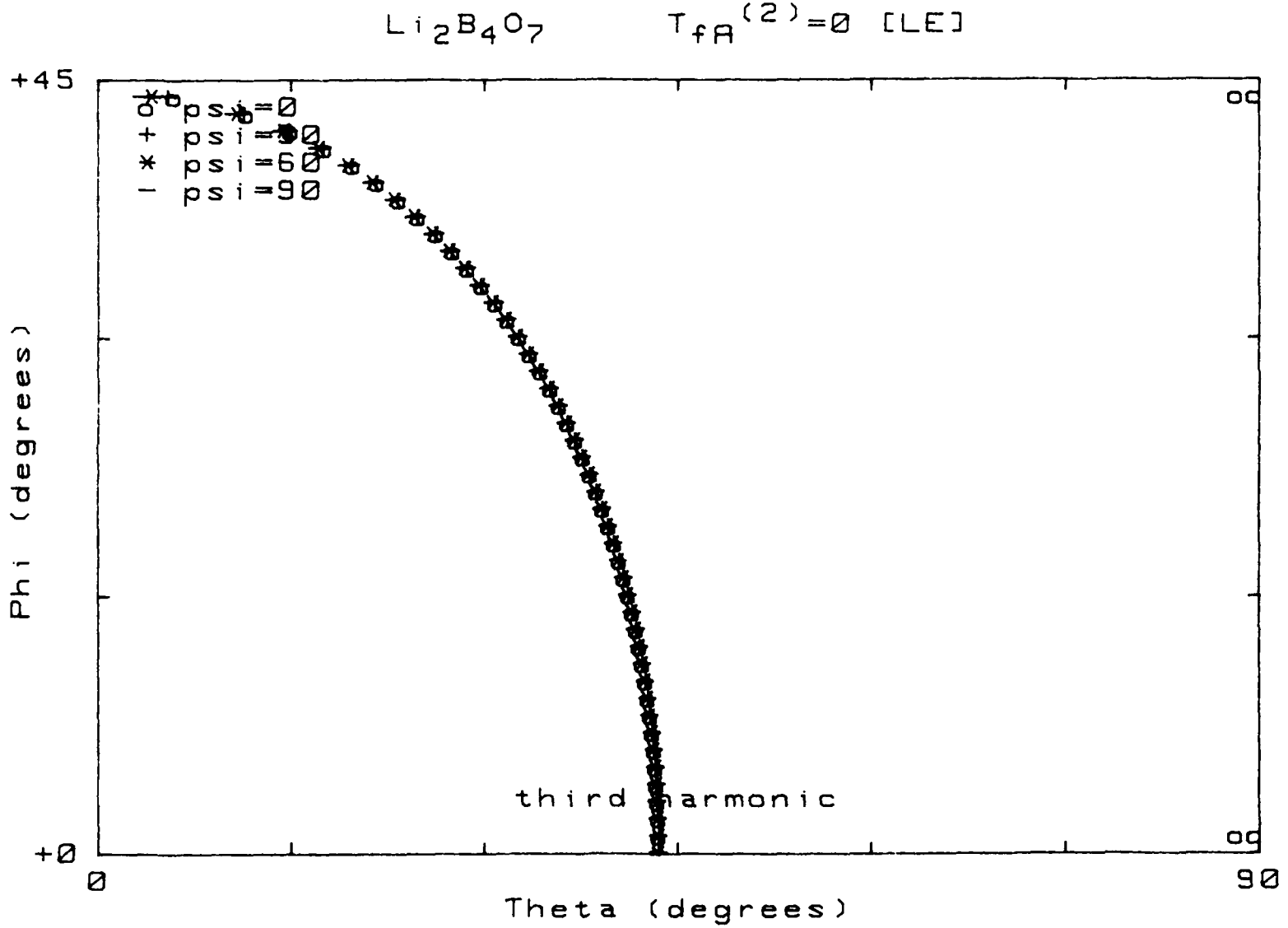

Figure 44. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M = 3; mode "a"; psi=0° (30°)90°; [LE]

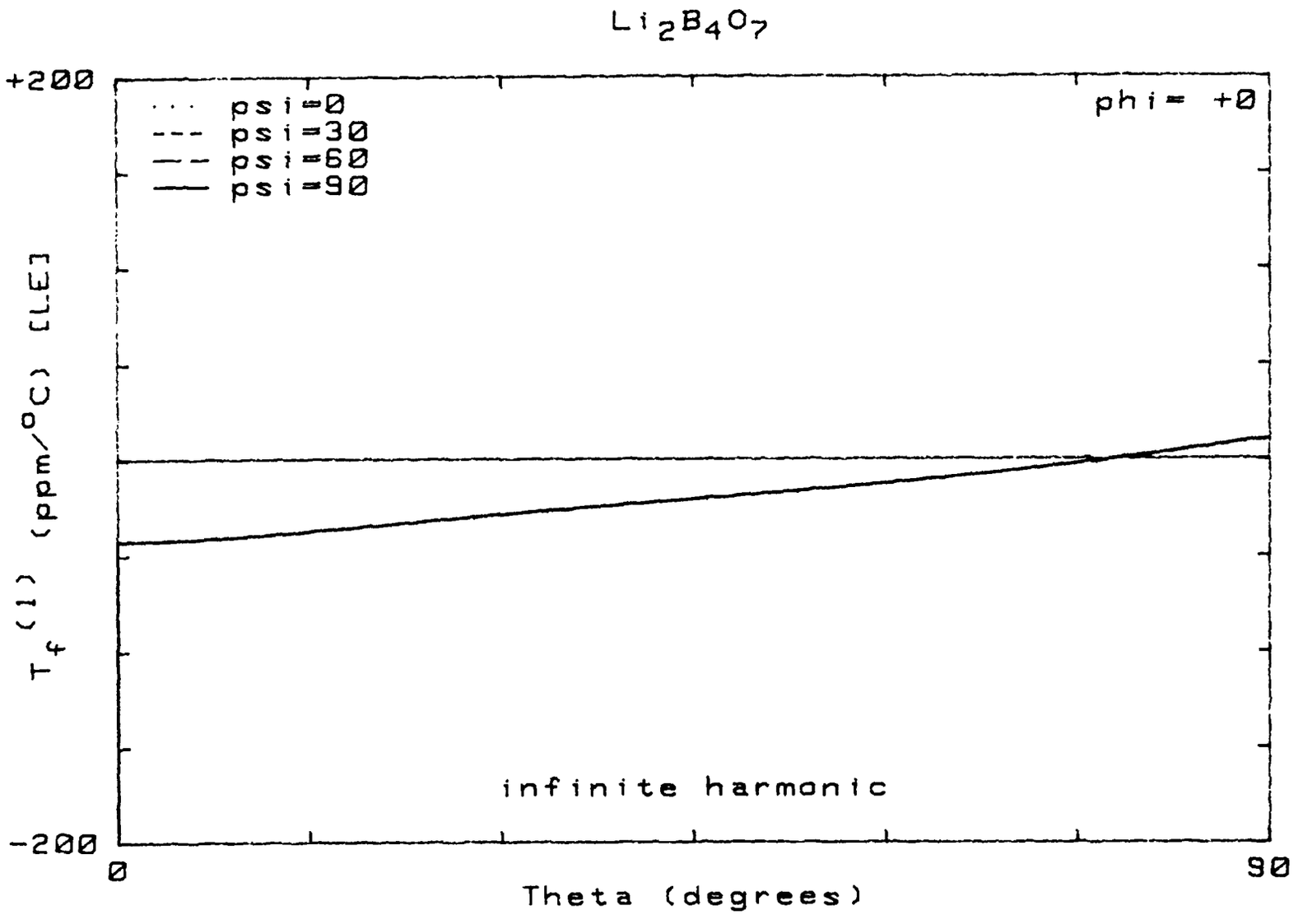

Figure 45. TC(1) for (yxwl)ϕ=0°/θ cuts; M = ∞; mode "a"; psi=0° (30°)90°; [LE]

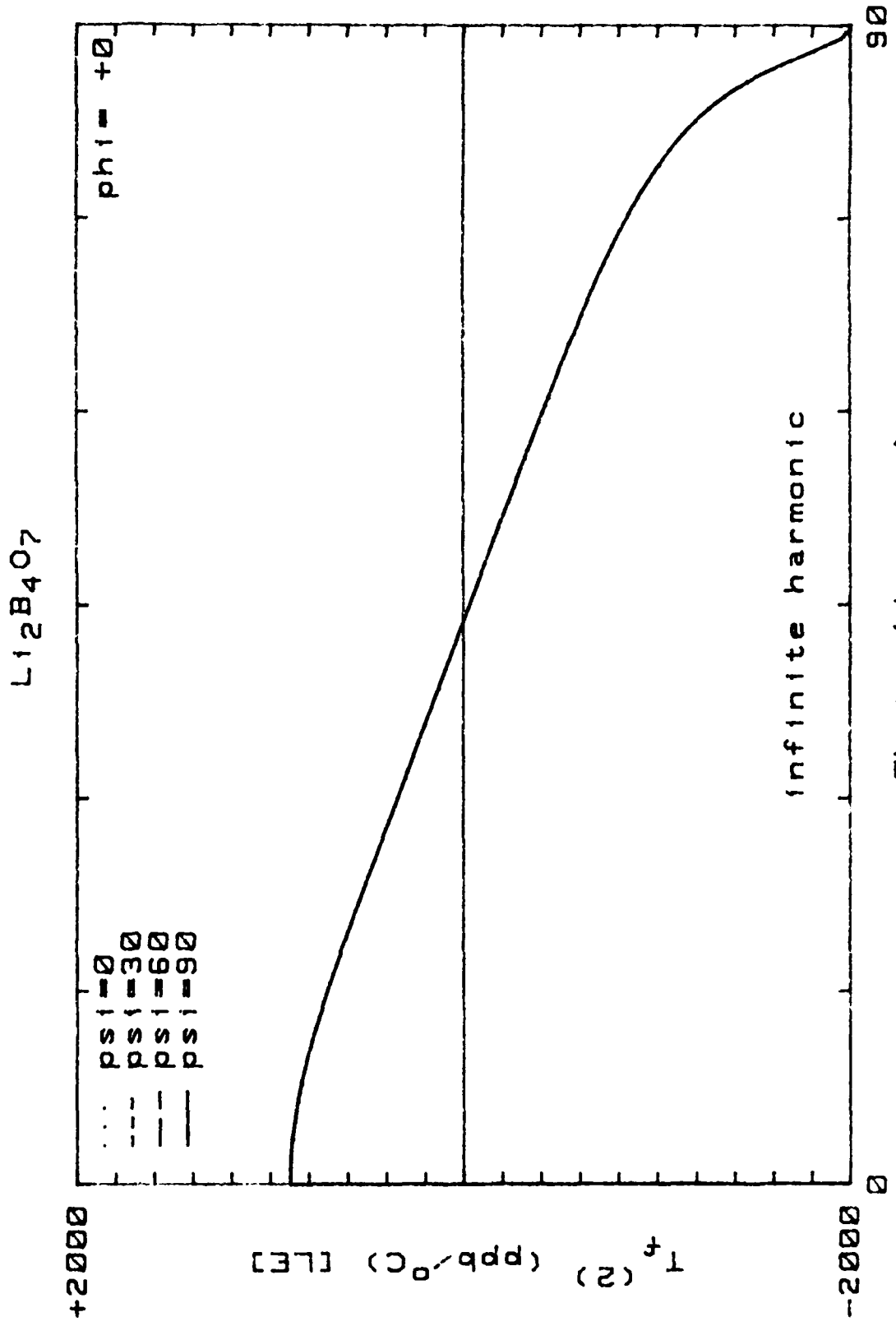

Figure 46. TC(2) for (yxw)Φ=0°/Θcuts; M =∞; mode "a"; psi=0°(30°)90°; [LE]

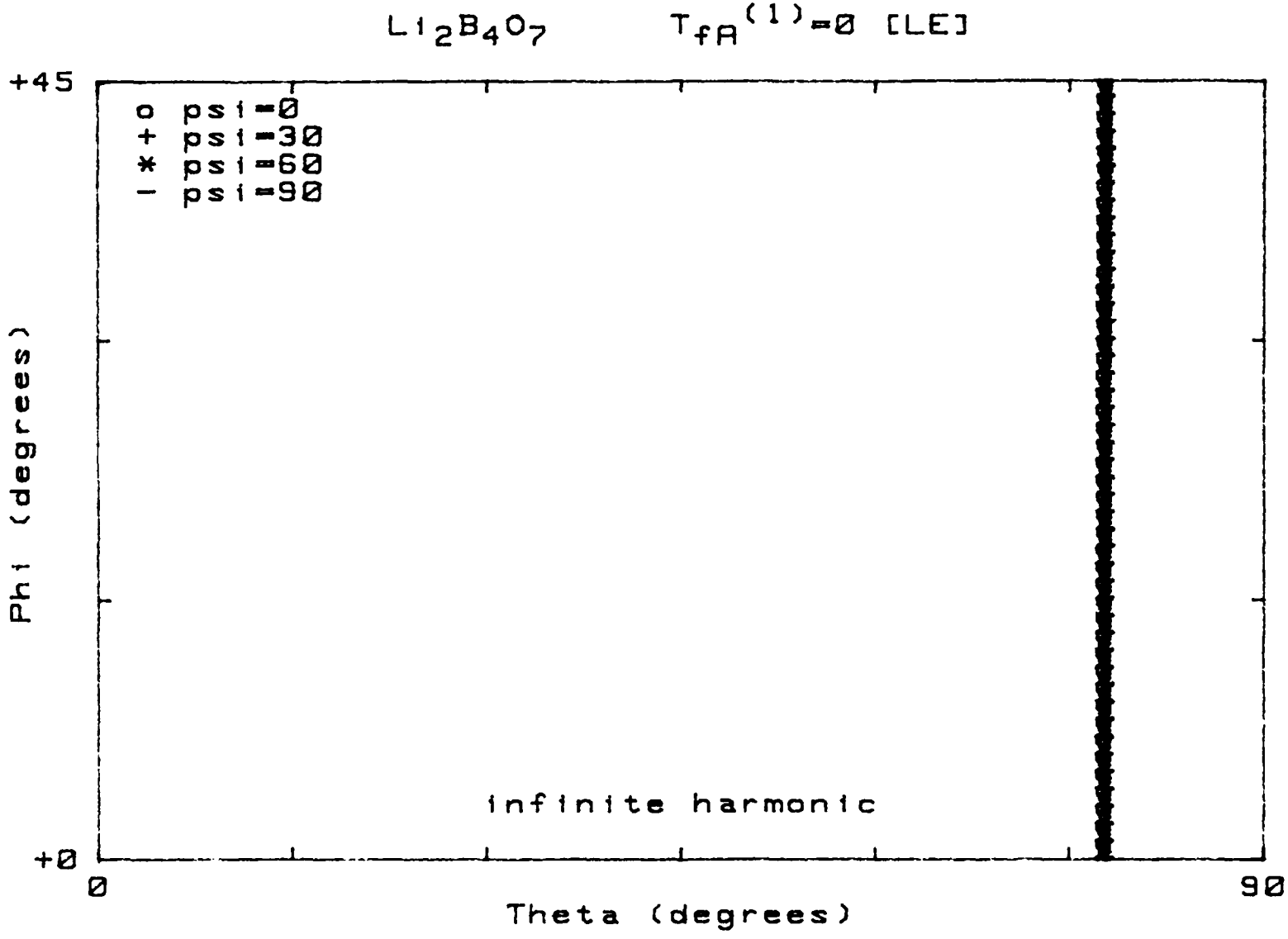

Figure 47. Locus of TC(1)=0 for (yxwl)ϕ/θcuts; M =∞; mode "a"; psi=0°(30°)90°; [LE]

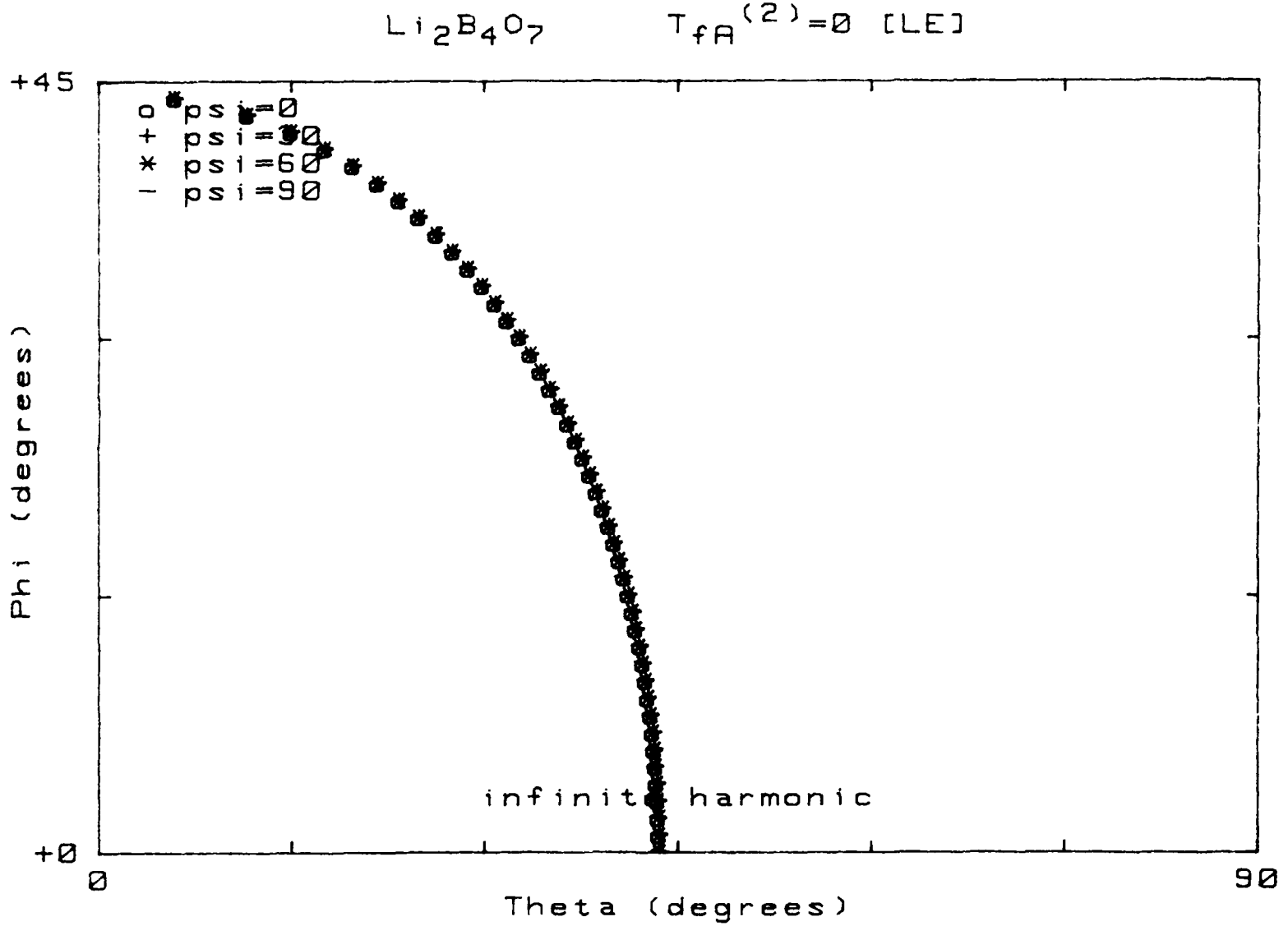

Figure 48. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M =∞ ; mode "a"; psi=0°(30°)90°; [LE]

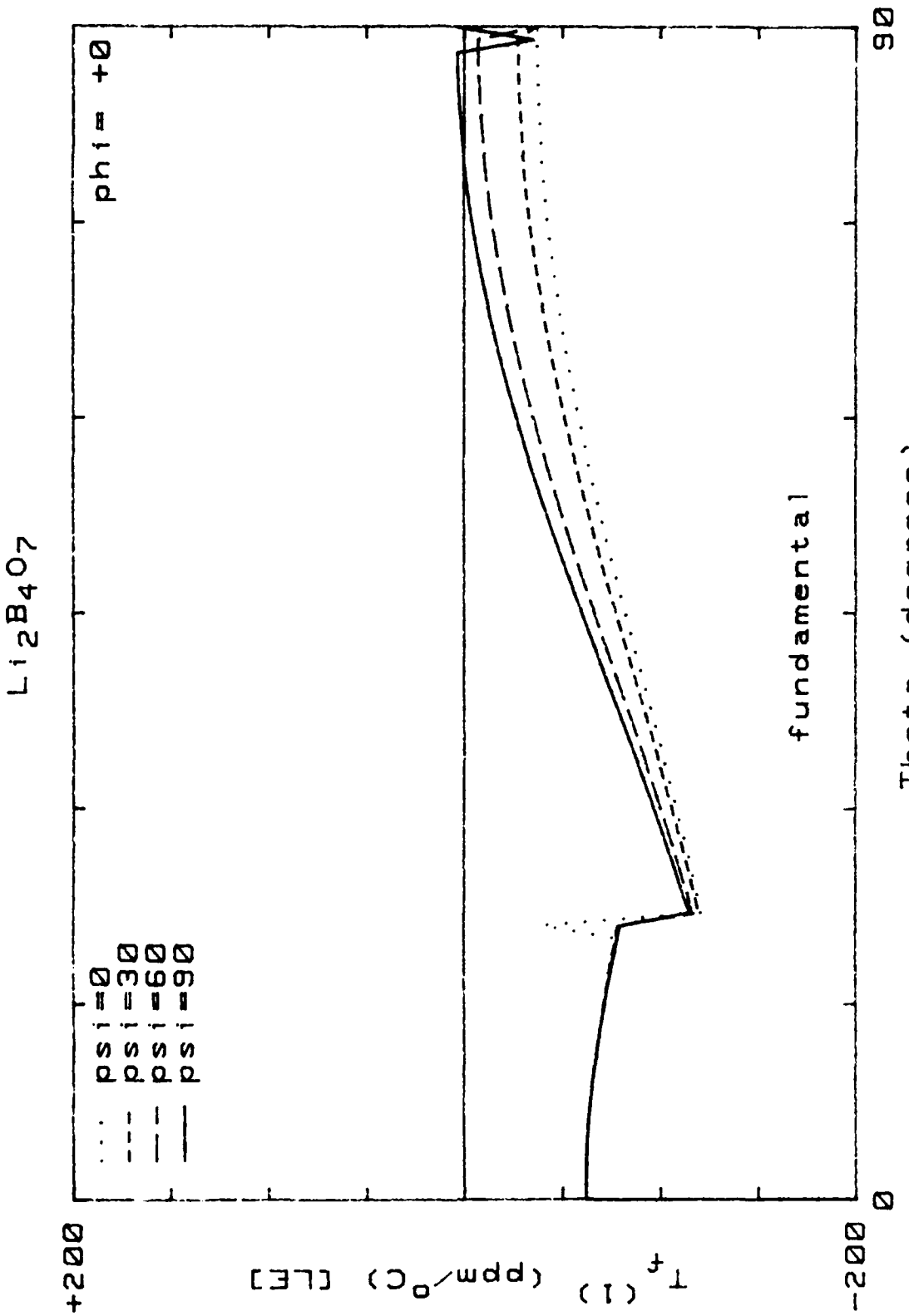

Figure 49. TC(1) for (yxwl)ϕ=0°/θ cuts; M = 1; mode "b"; psi=0°(30°)90°; [LE]

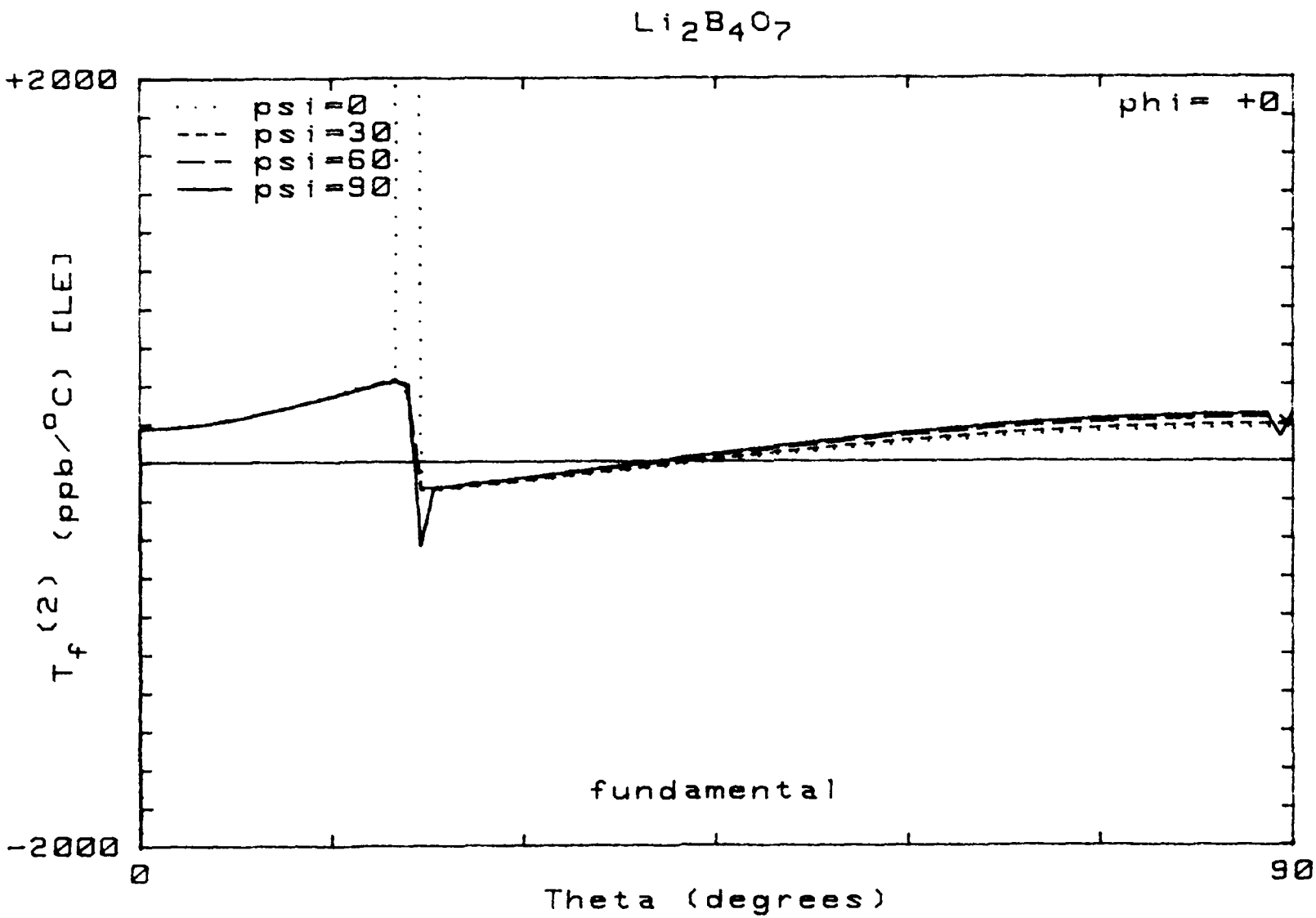

Figure 50. TC(2) for (yxwl)ϕ=0°/θ cuts; M = 1; mode "b"; psi=0°(30°)90°; [LE]

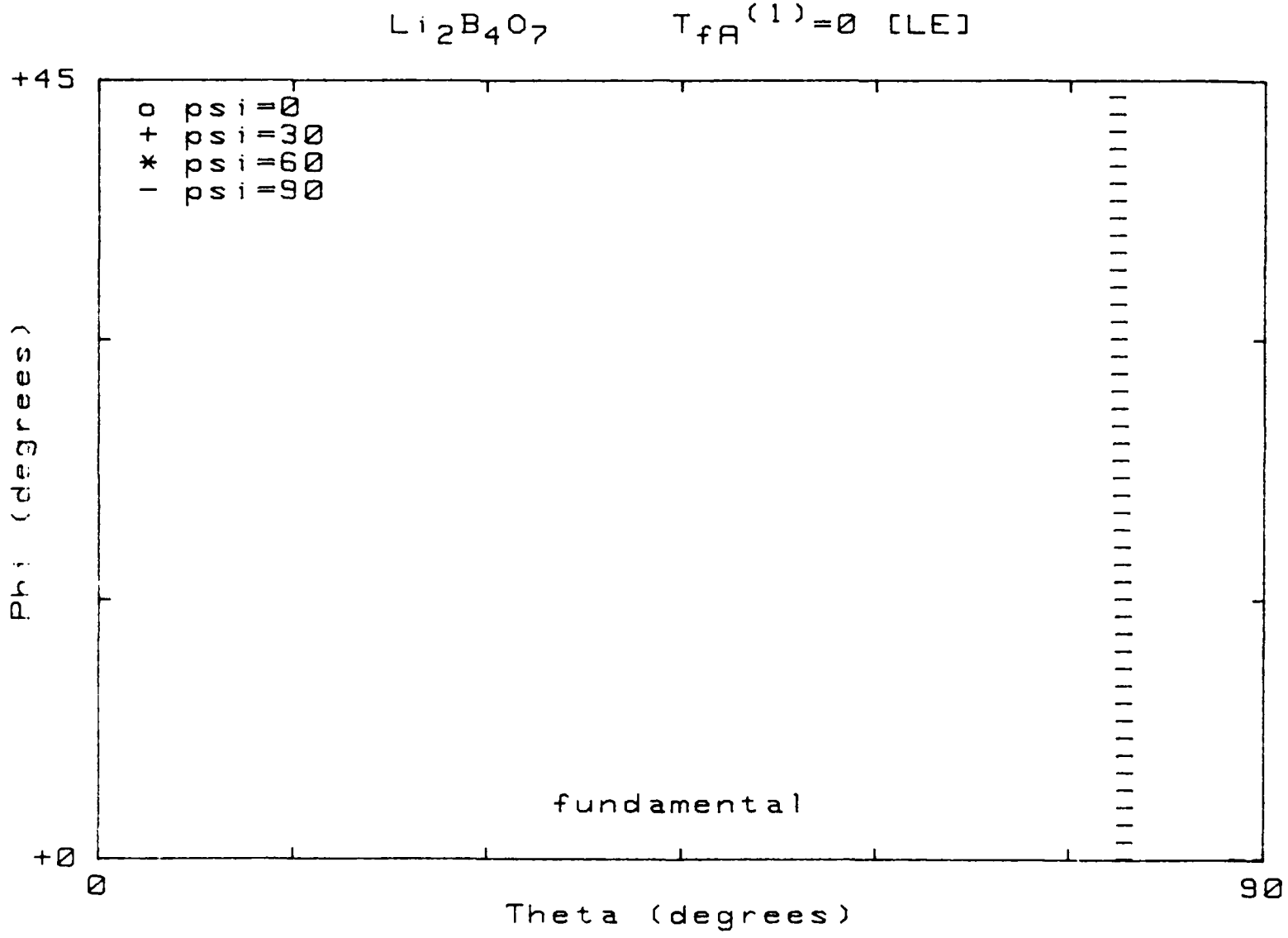

Figure 51. Locus of TC(1)=0 for (yxwl)ϕ/θcuts; M = 1; mode "b"; psi=0°(30°)90°; [LE]

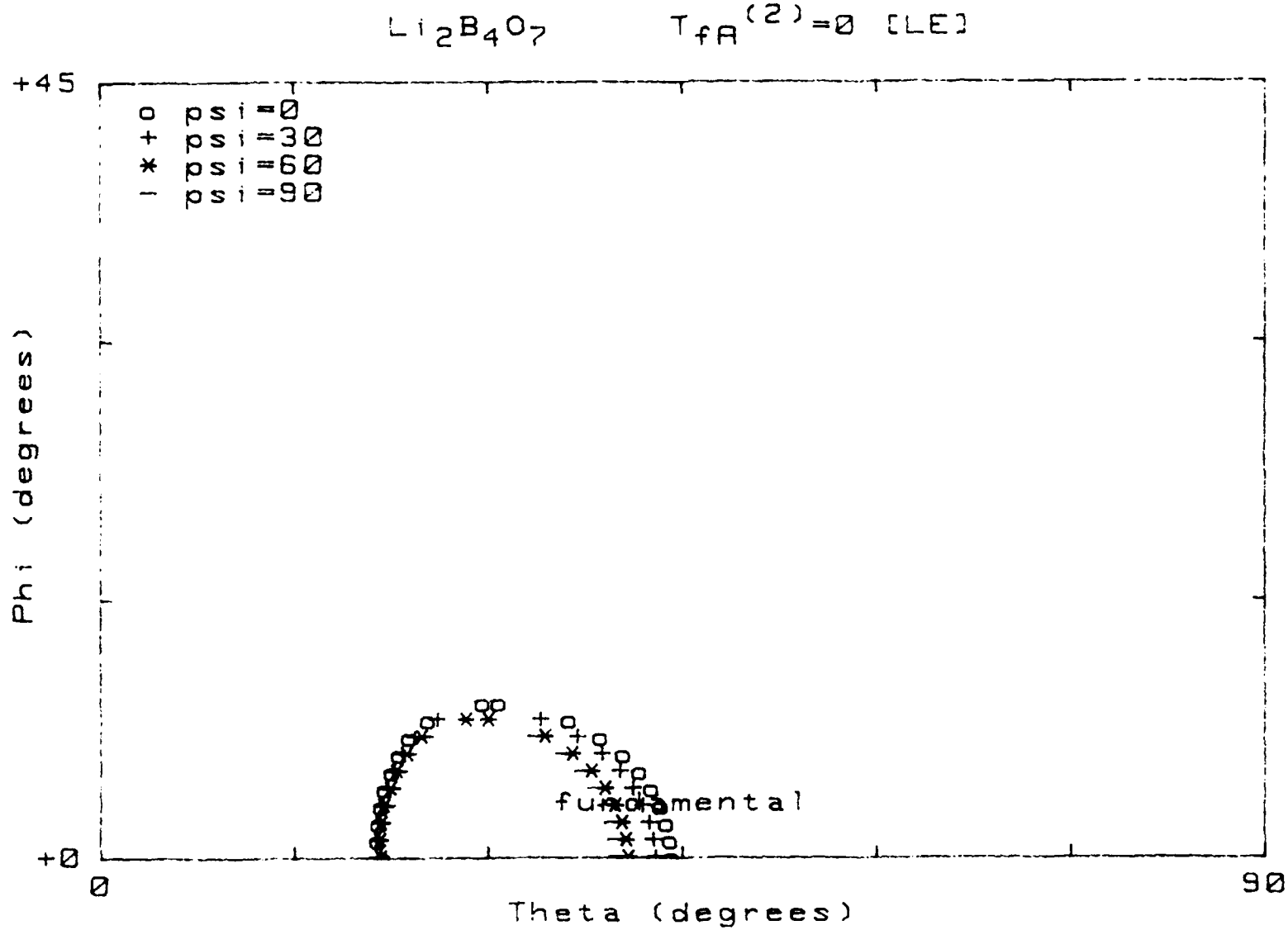

Figure 52. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M = 1; mode "b"; psi=0°(30°)90°; [LE]

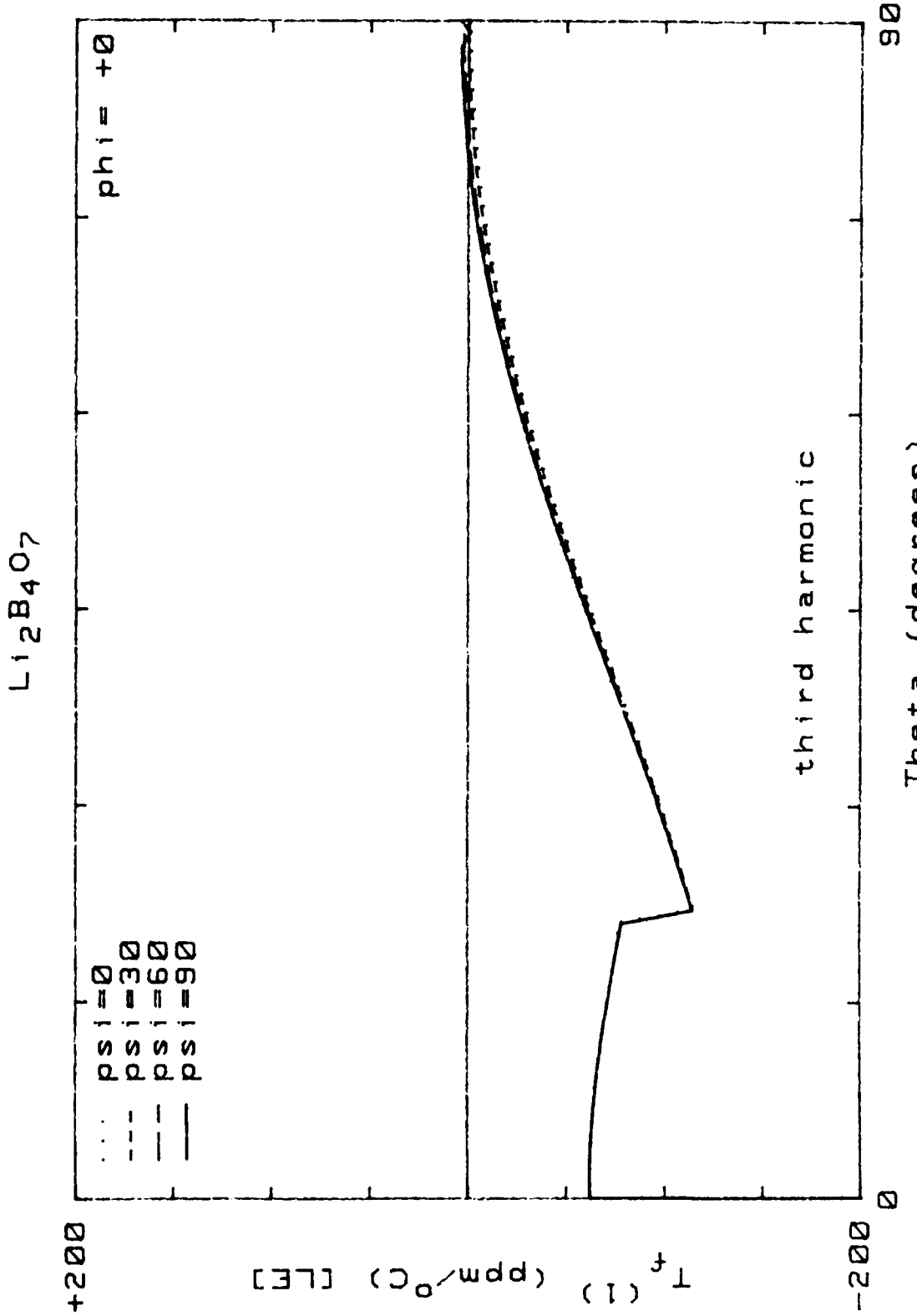

Figure 53. TC(1) for (yxwl)ϕ=0°/θ cuts; M = 3; mode "b"; psi=0°(30°)90°; [LE].

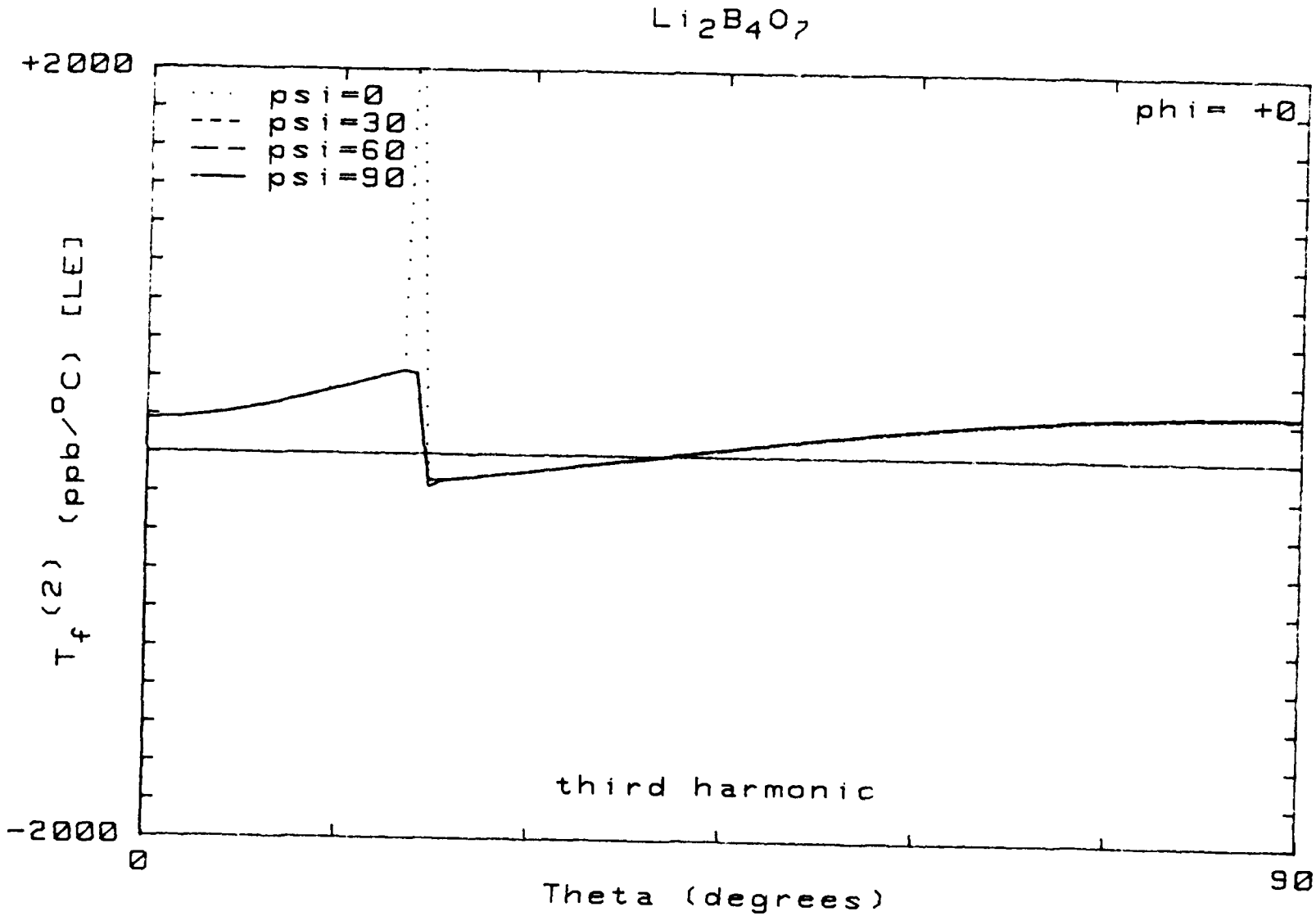

Figure 54. TC(2) for (yxwl)ϕ=0°/θ cuts; M = 3; mode "b"; psi=0°(30°)90°; [LE]

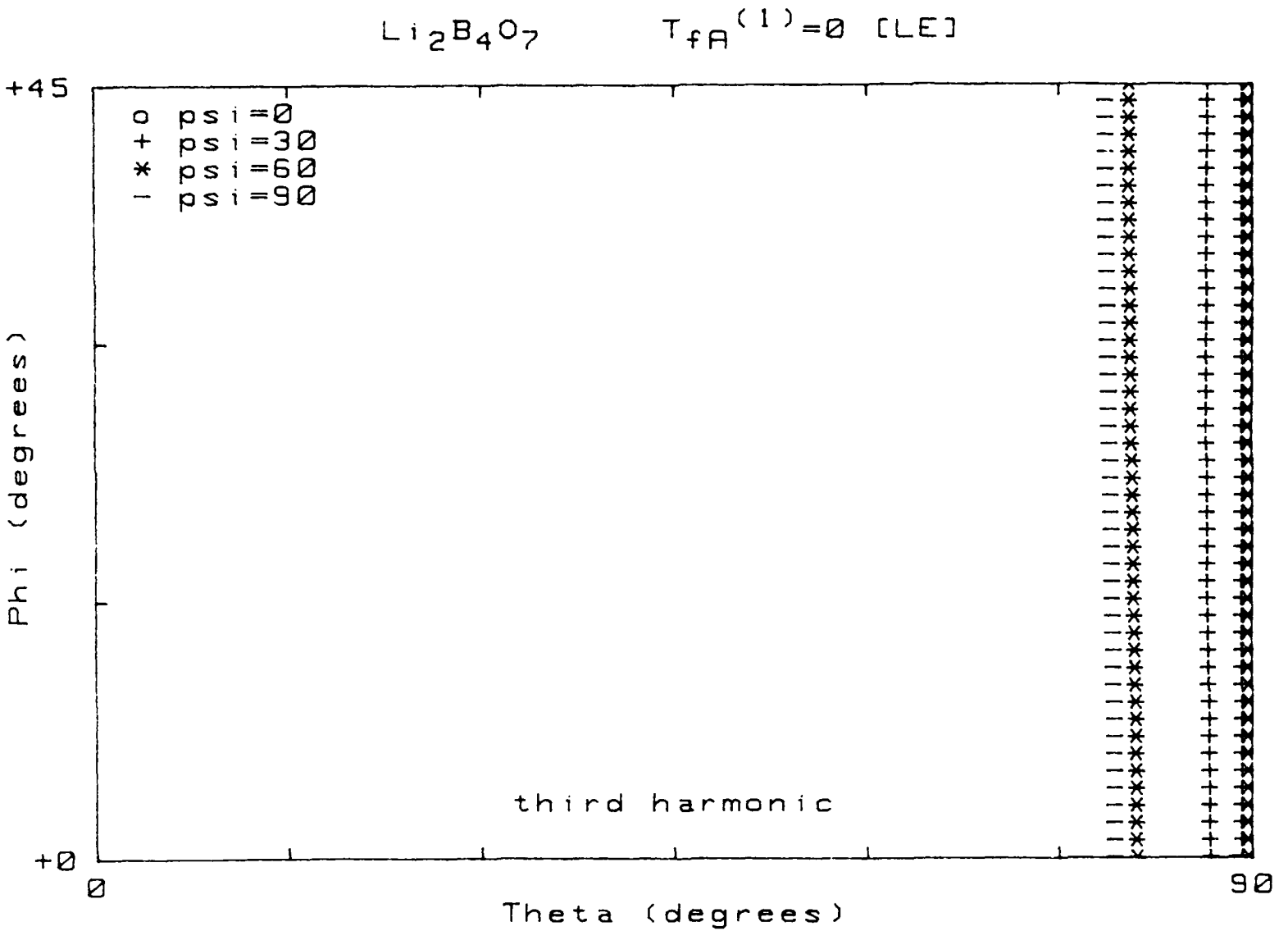

Figure 55. Locus of TC(1)=0 for (yxwl)ϕ/θ cuts; M = 3; mode "b"; psi=0°(30°)90°; [LE].

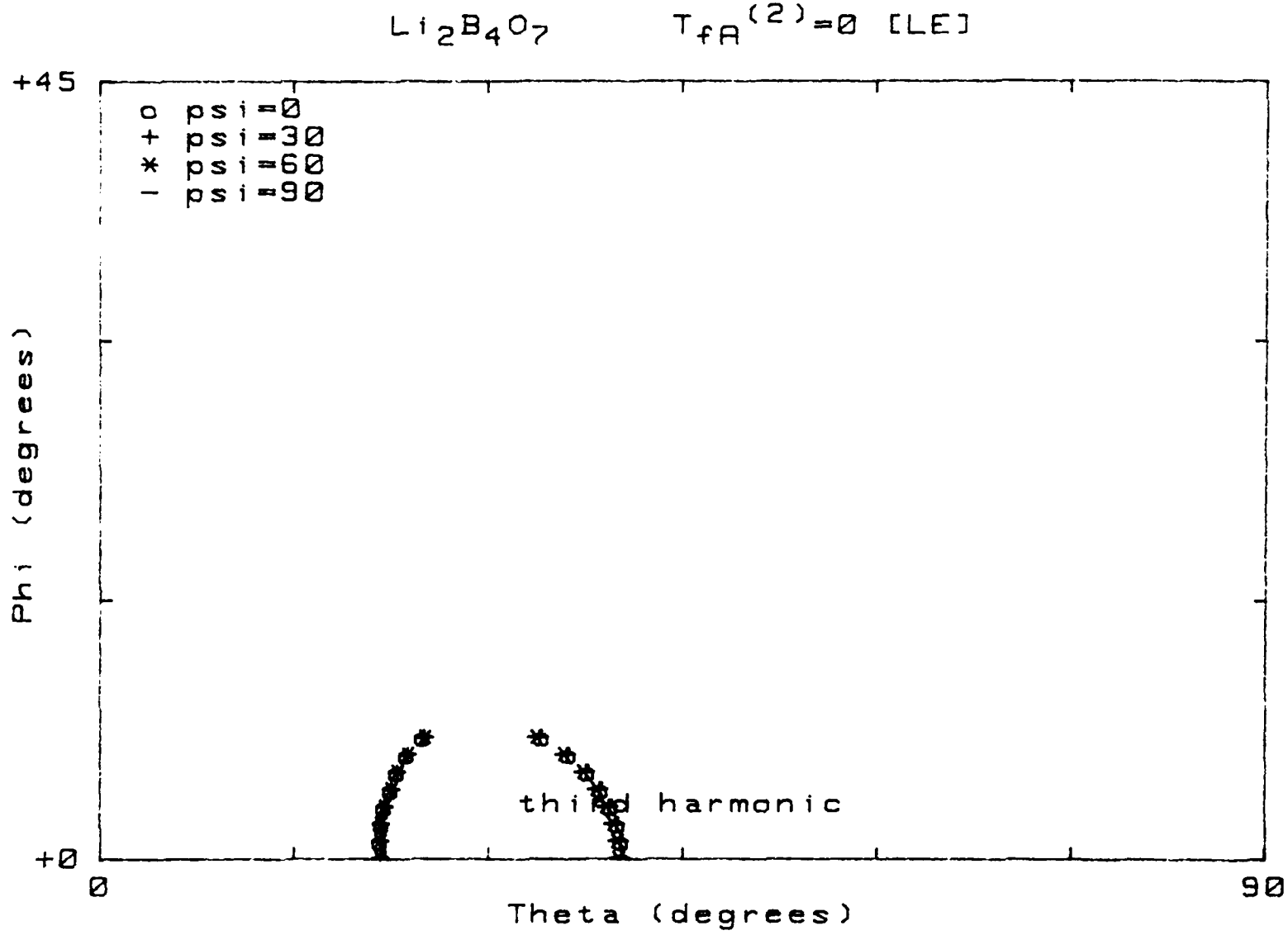

Figure 56. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M = 3; mode "b"; psi=0°(30°)90°; [LE].

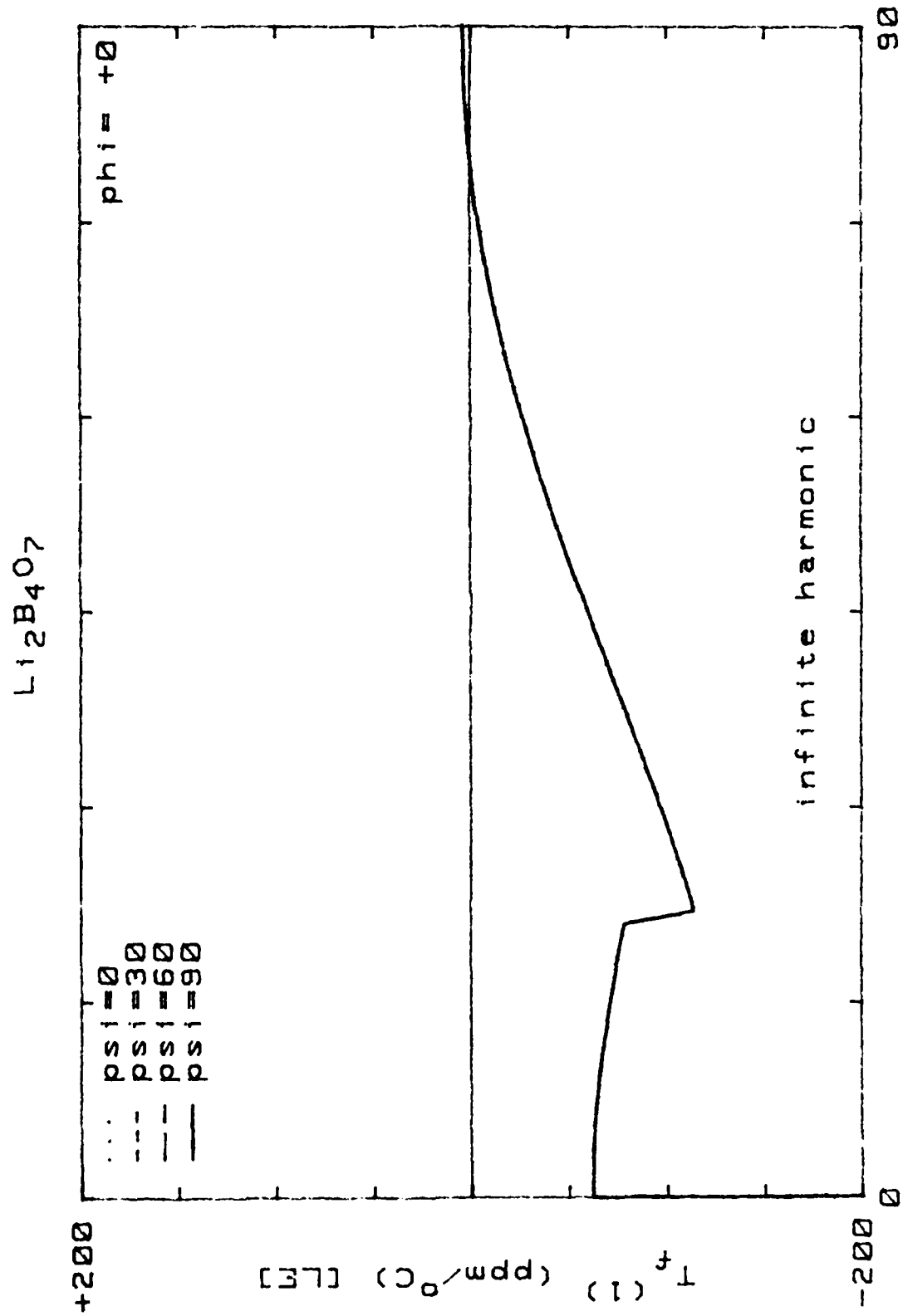

Figure 57. TC(1) for (yxwl)ϕ=0°/θ cuts; M =∞ ; mode "b"; psi=0°(30°)90°; [LE].

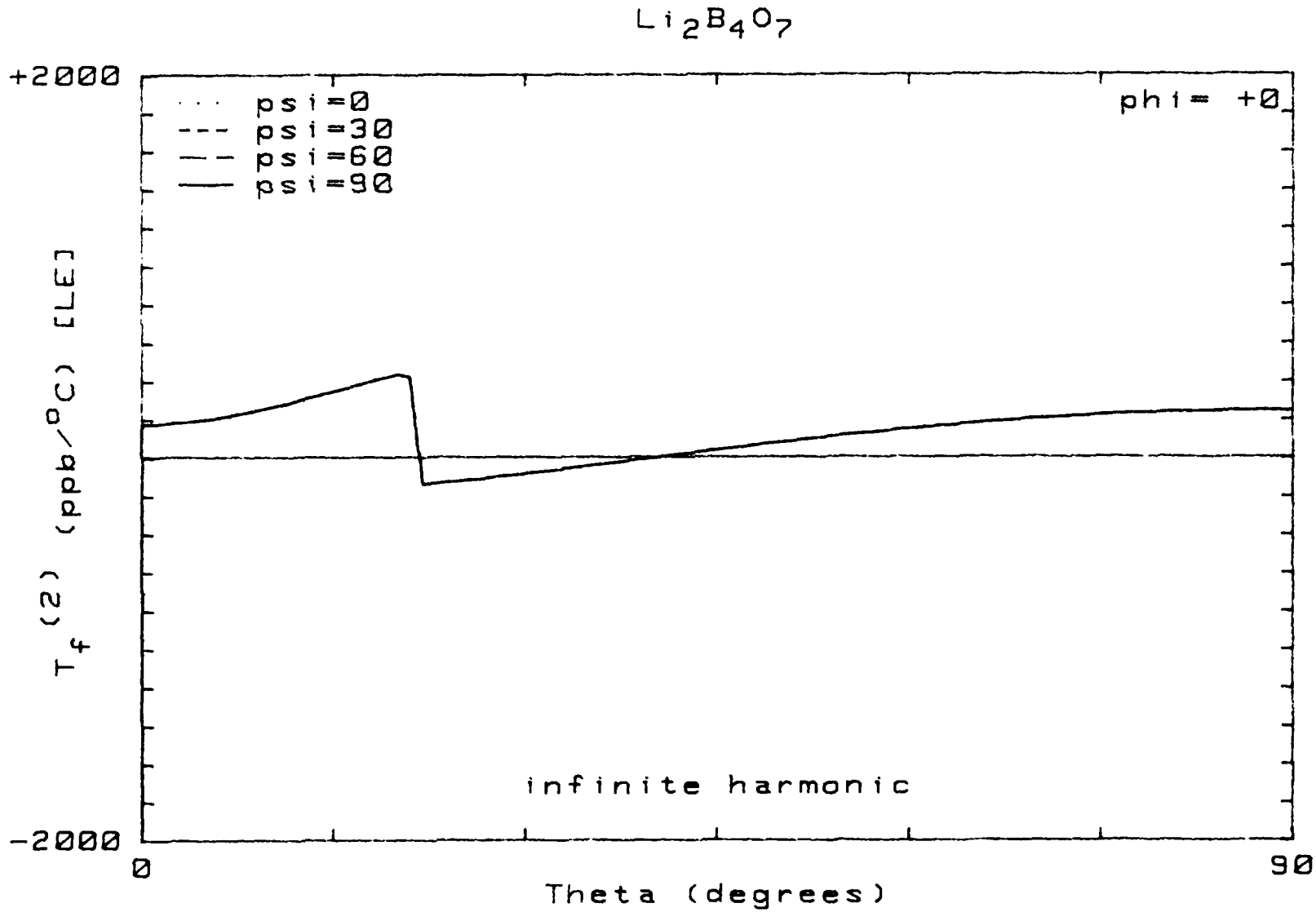

Figure 58. TC(2) for (yxwl)ϕ =0°/θ cuts; M =∞ ; mode "b"; psi=0°(30°)90°; [LE].

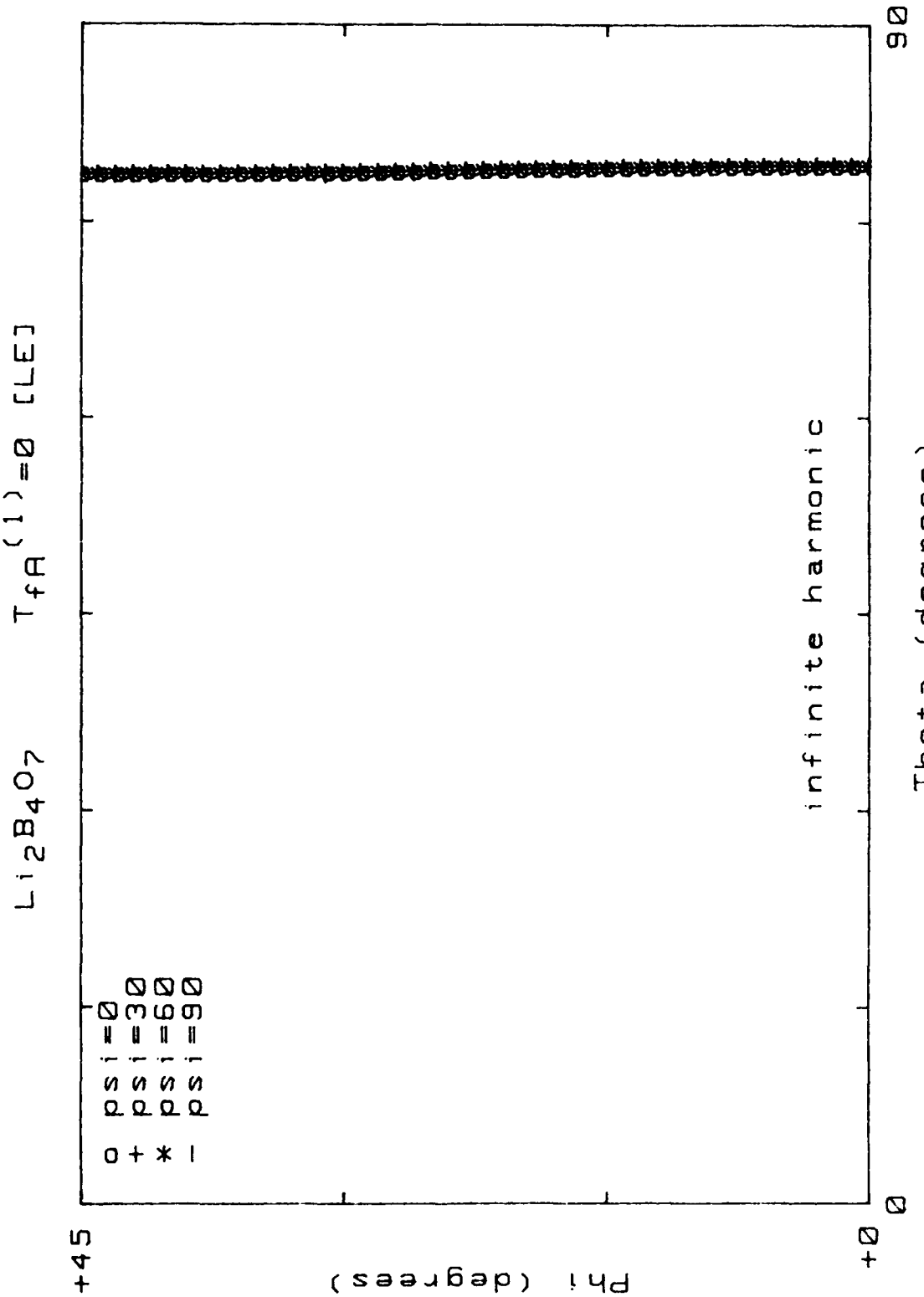

Figure 59. Locus of TC(1)=0 for (yxwl)ϕ/θ cuts; M =∞ ; mode "b"; psi=0°(30°)90°; [LE].

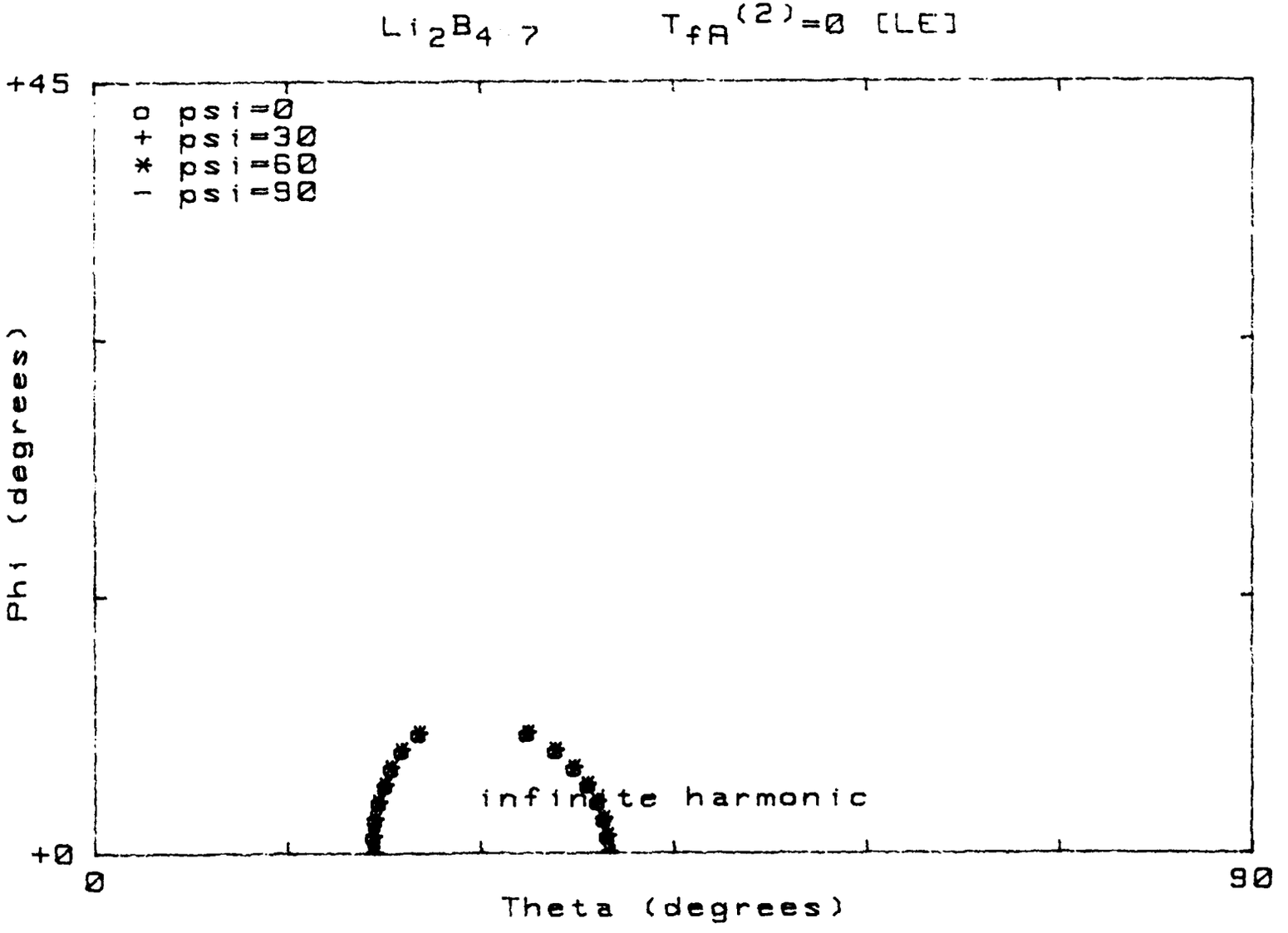

Figure 60. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M =∞ ; mode "b"; psi=0°(30°)90°; [LE].

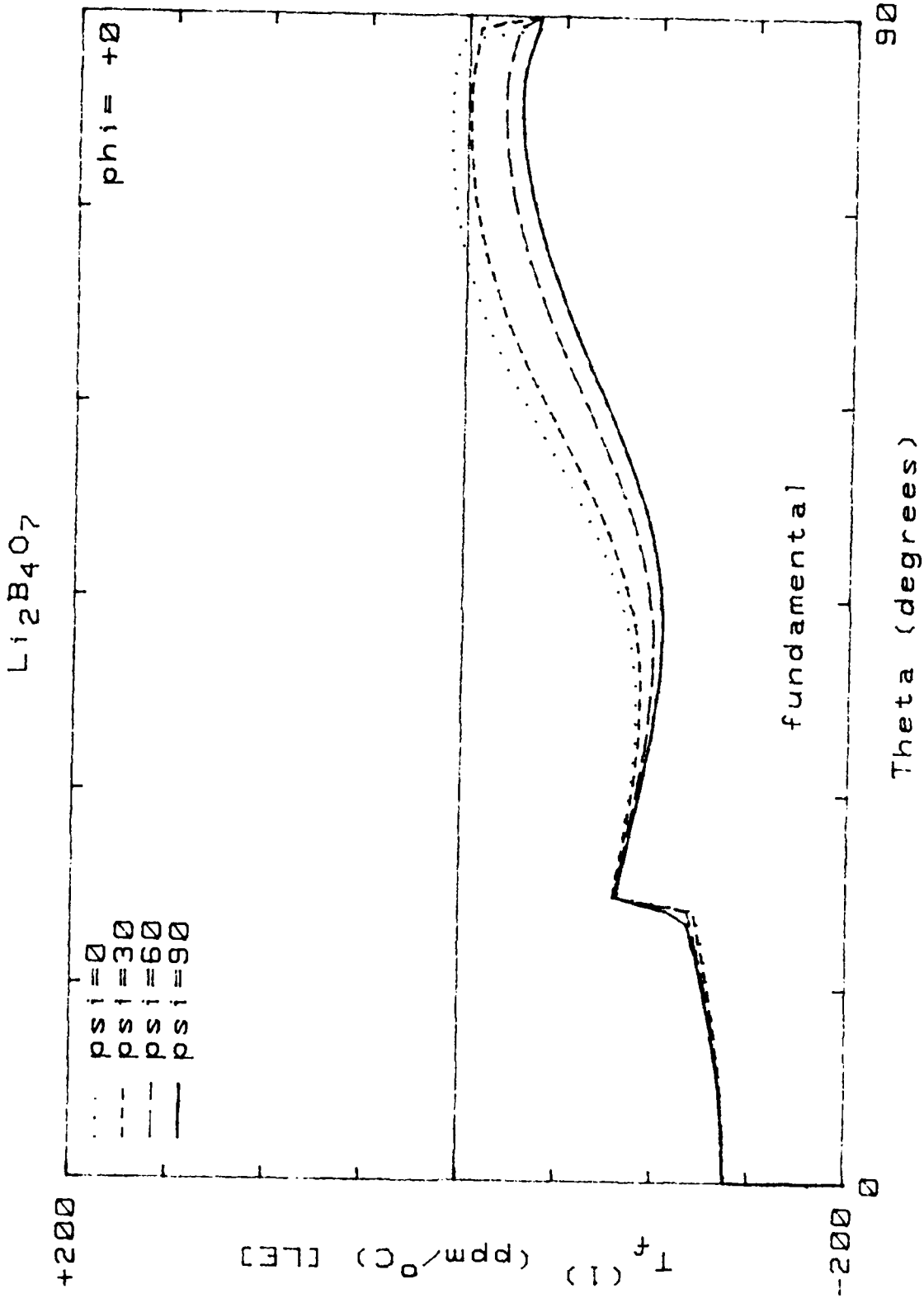

Figure 61. TC(1) for (yxwl)ϕ=0°/θ cuts; M = 1; mode "c"; psi=0°(30°)90°; [LE].

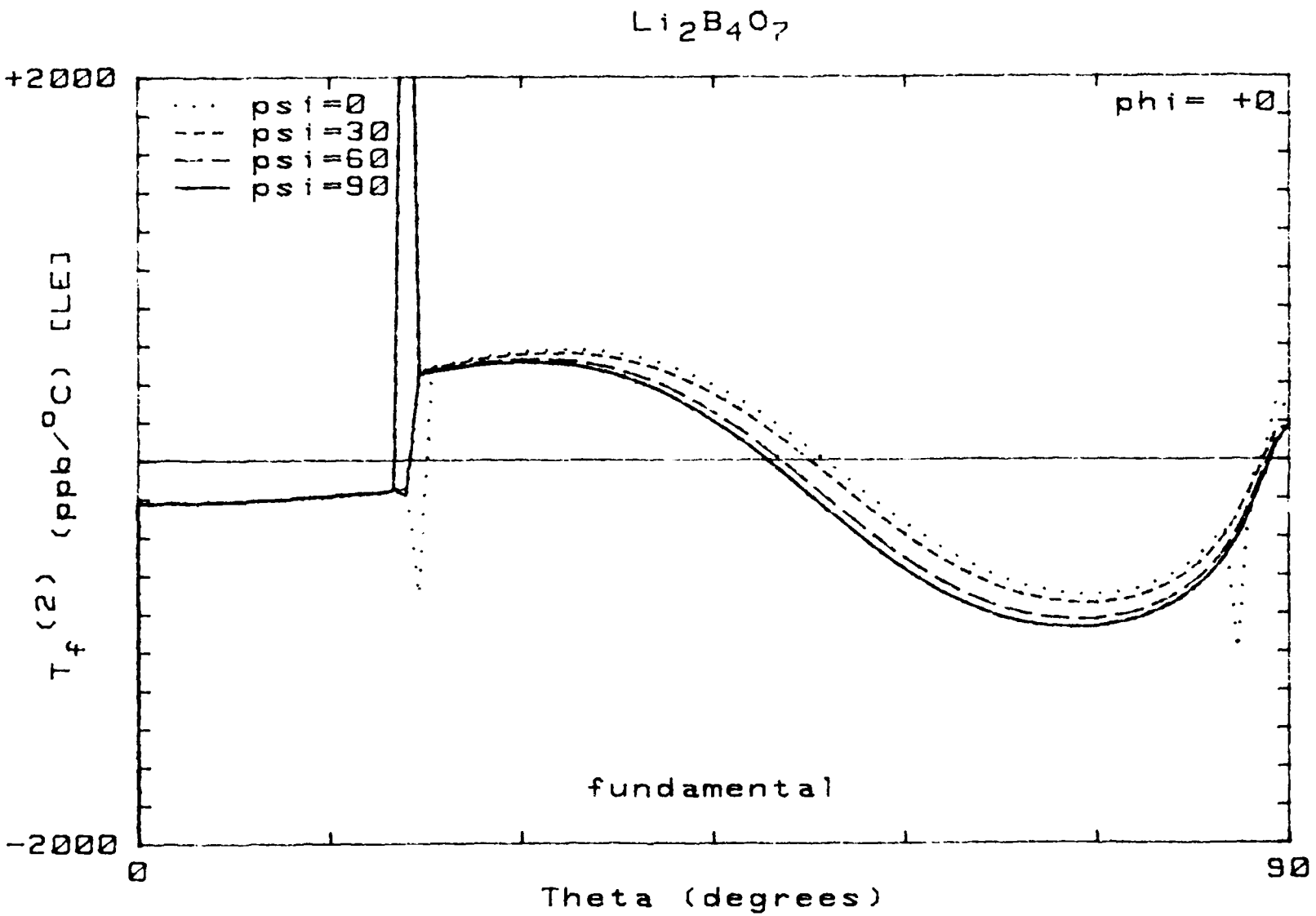

Figure 62. TC(2) for (yxwl)ϕ =0°/θ cuts; M = 1; mode "c"; psi=0°(30°)90°; [LE].

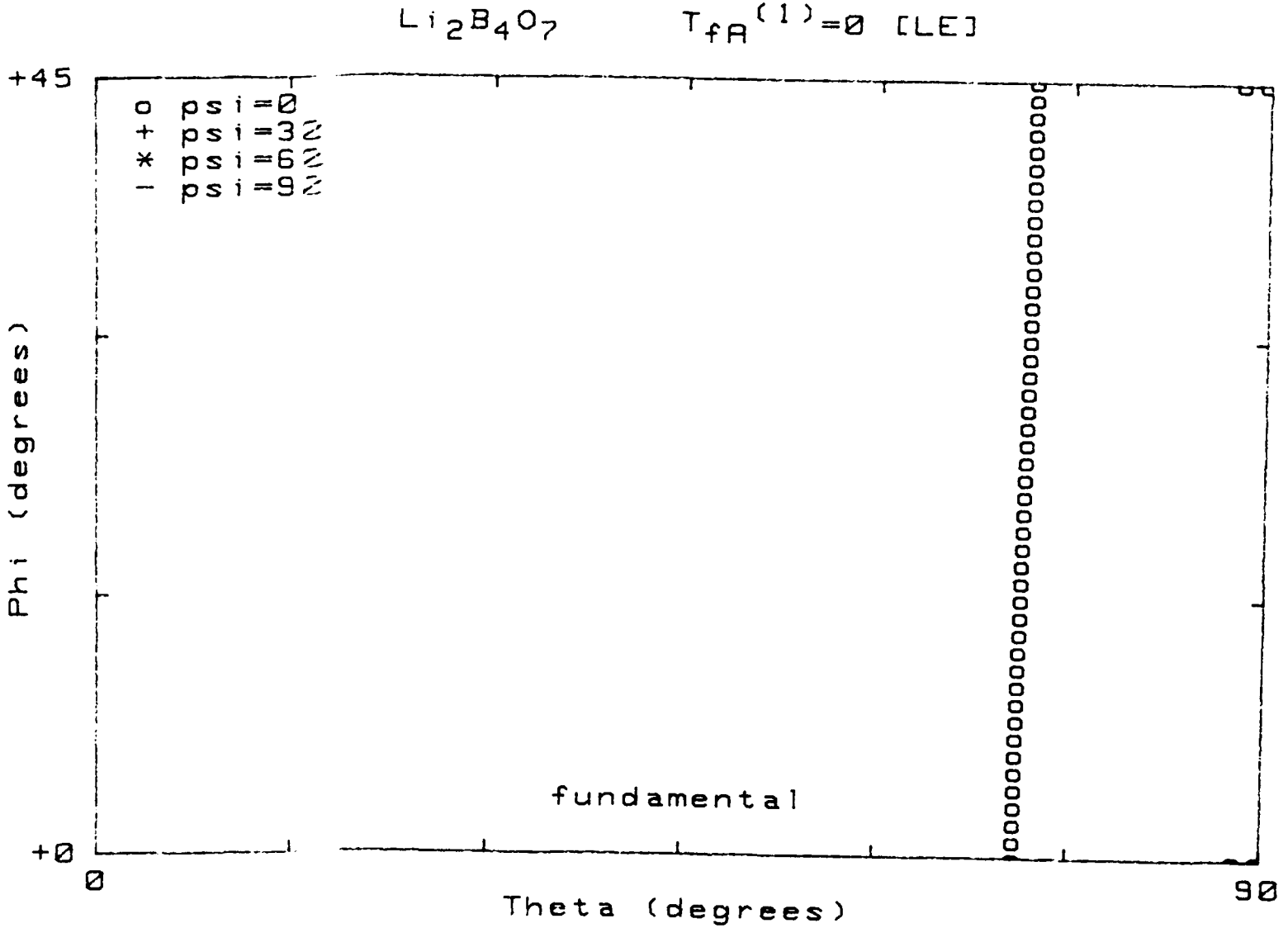

Figure 63. Locus of TC(1)=0 for (yxwl) ϕ/θ cuts; M = 1; mode "c"; psi=0°(30°)90°; [LE].

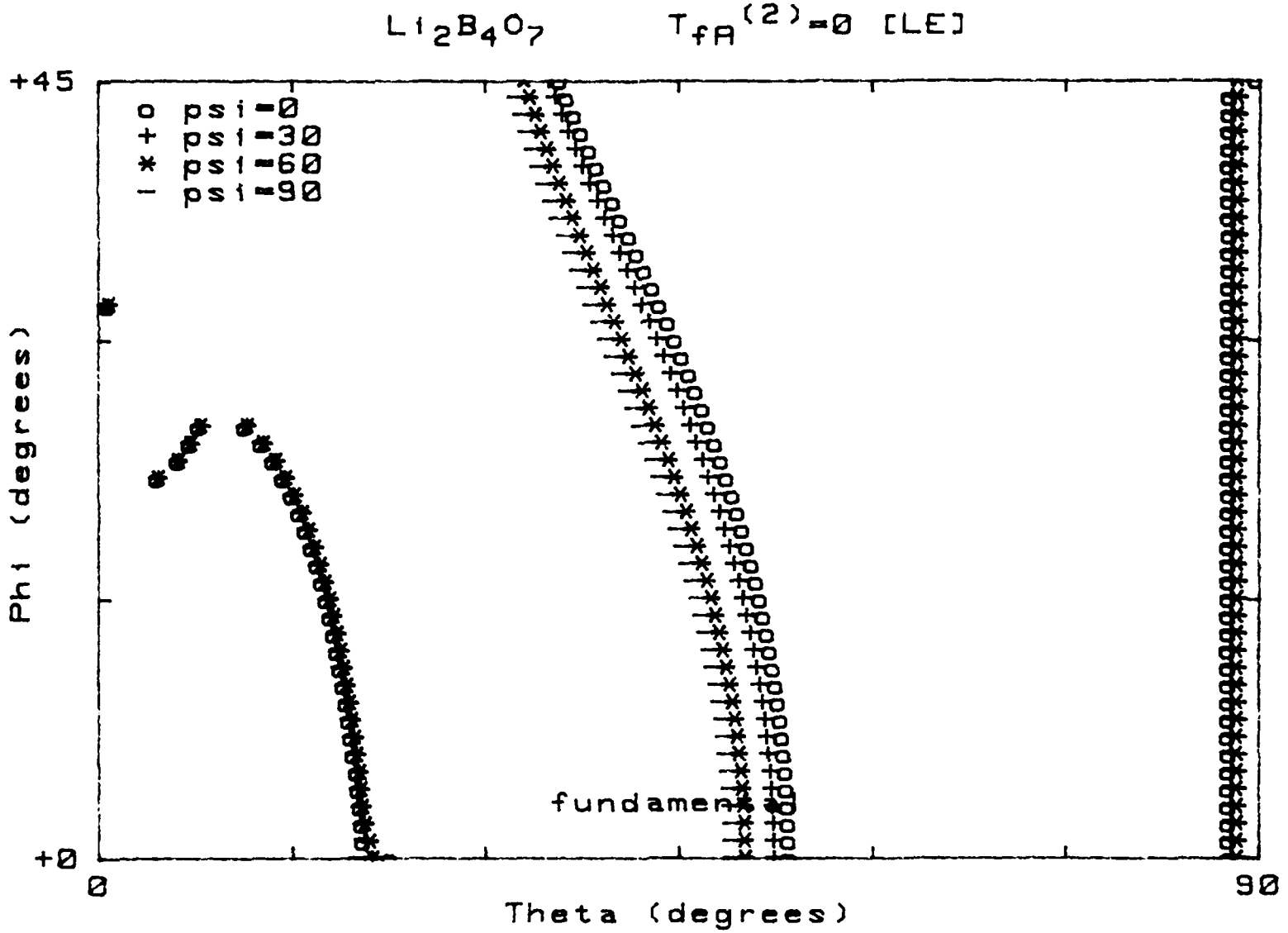

Figure 64. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M = 1; mode "c"; psi=0°(30°)90°; [LE].

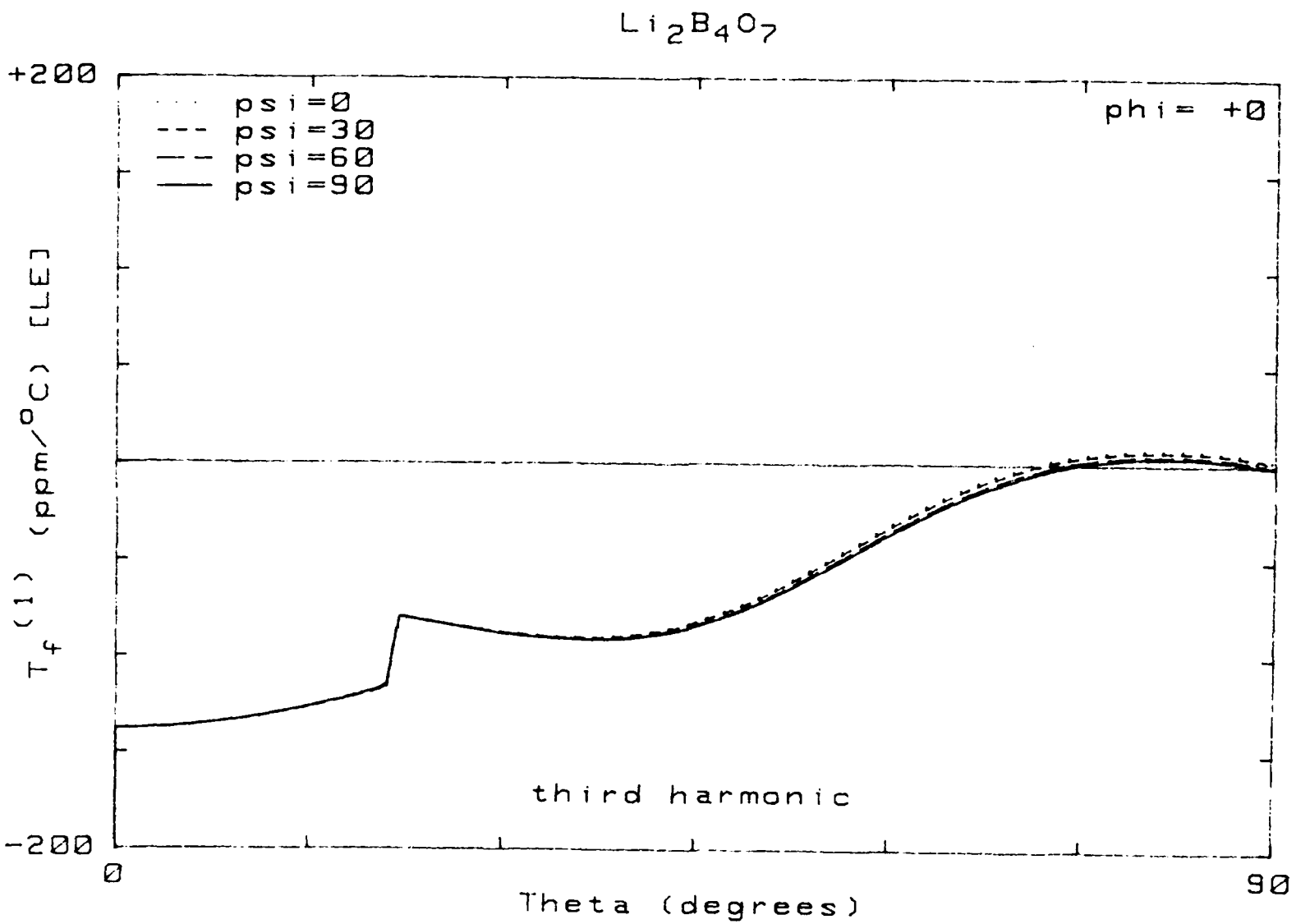

Figure 65. TC(1) for (yxwl)ϕ =0°/θ cuts; M = 3; mode "c"; psi=0°(30°)90°; [LE].

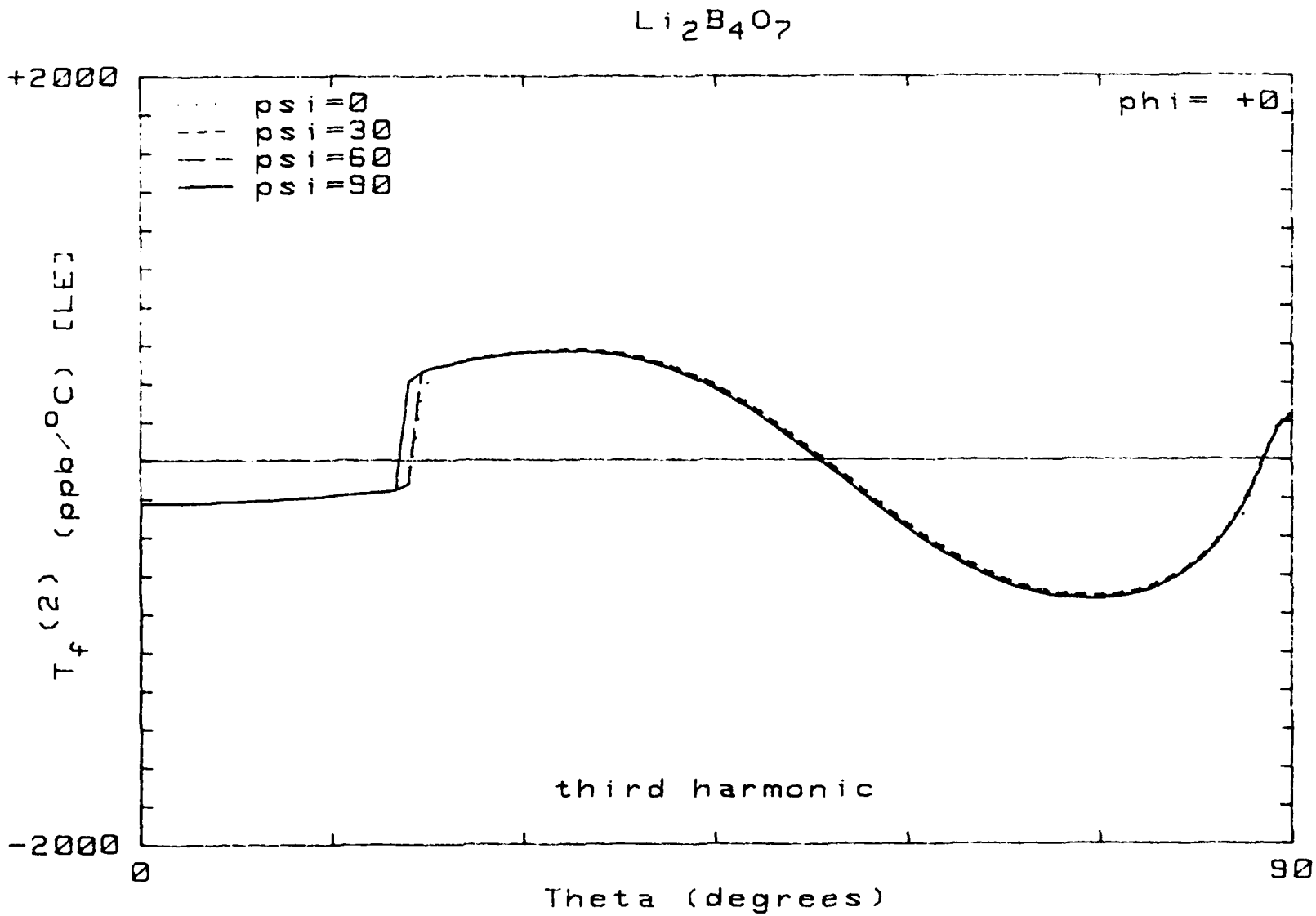

Figure 66. TC(2) for (yxwl)ϕ=0°/θ cuts; M = 3; mode "c"; psi=0°(30°)90°; [LE].

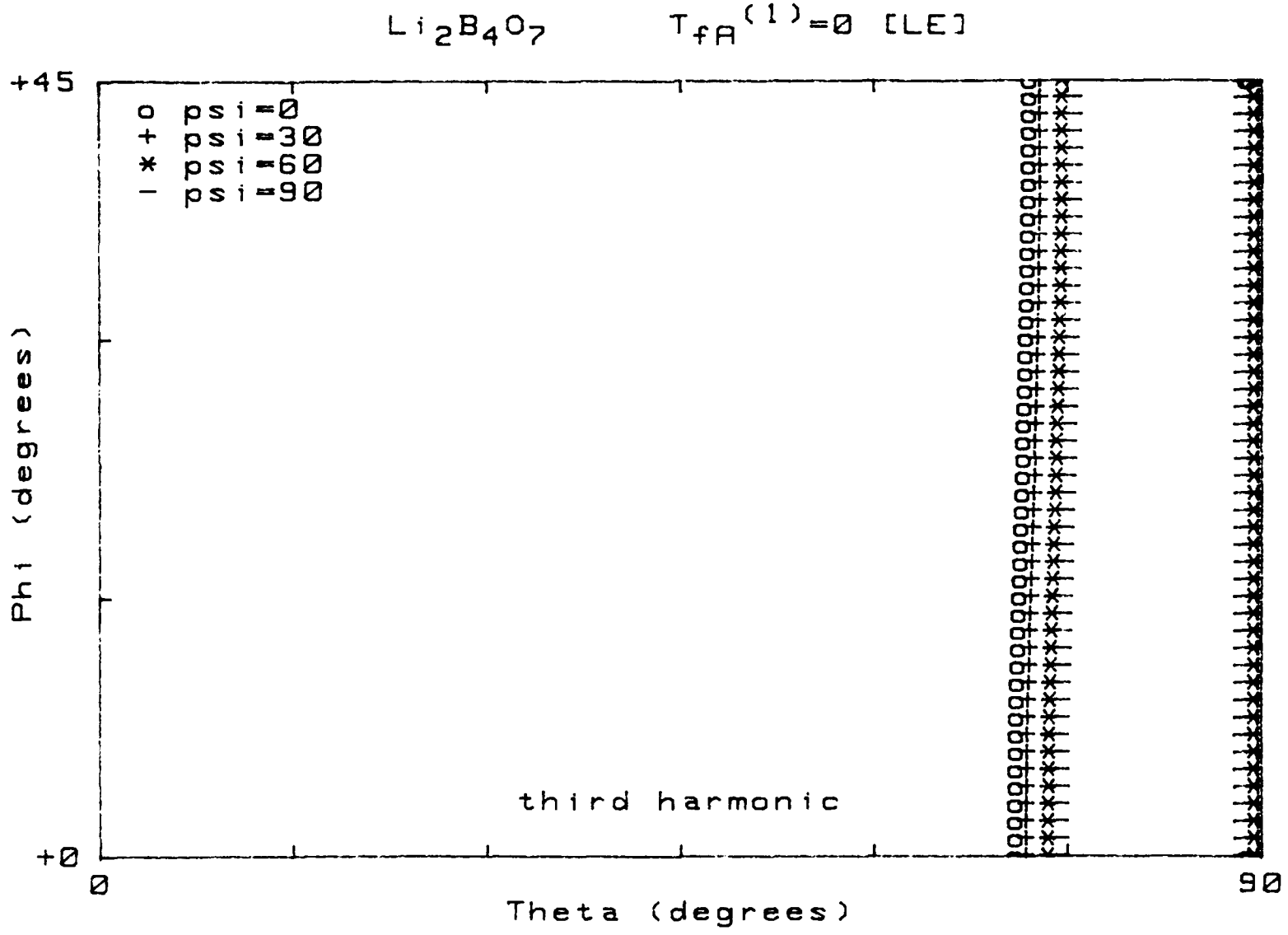

Figure 67. Locus of TC(1)=0 for (yxwl)ϕ/θ cuts; M = 3; mode "c"; psi=0°(30°)90°; [LE].

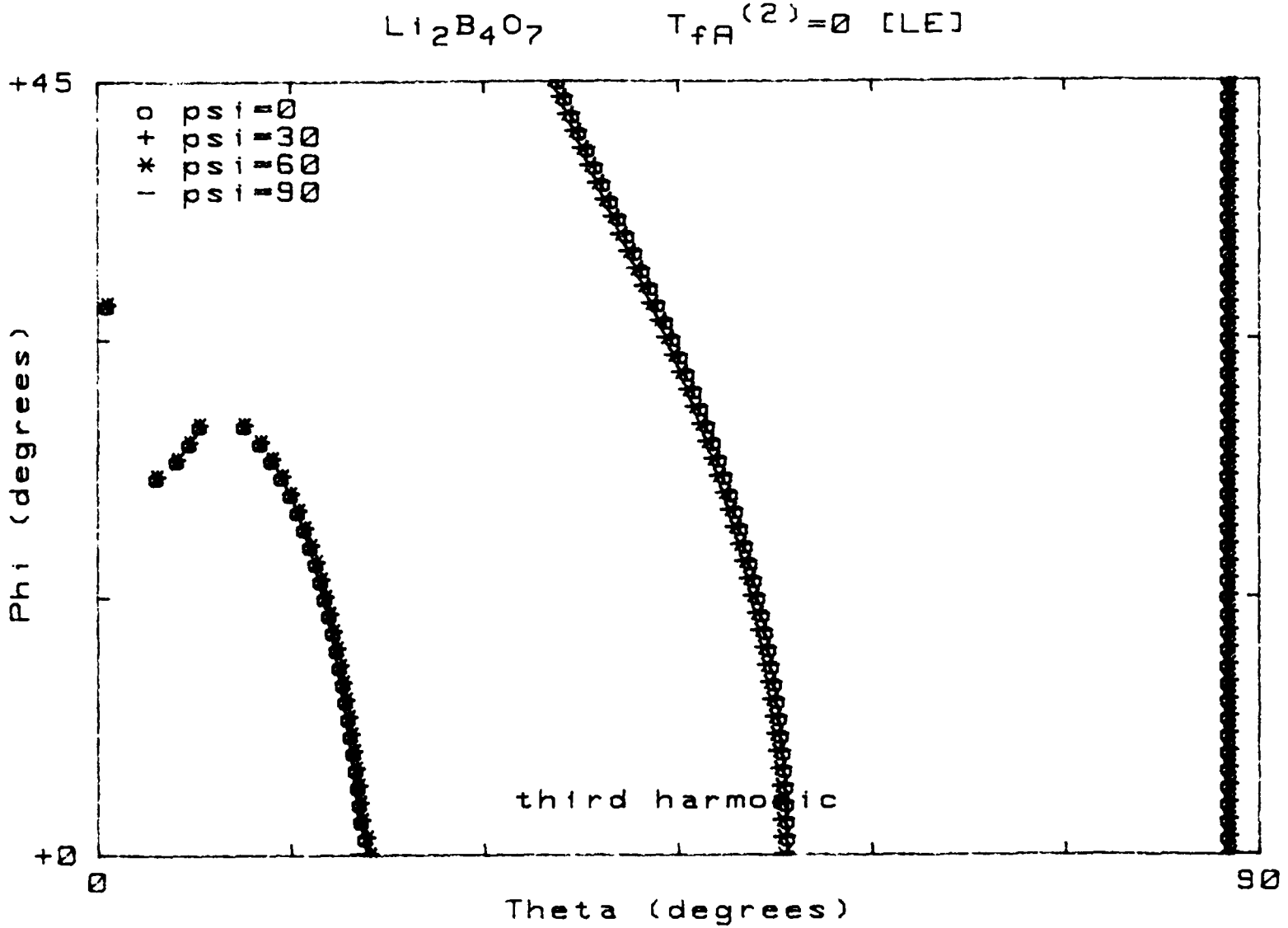

Figure 68. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M = 3; mode "c"; psi=0°(30°)90°; [LE].

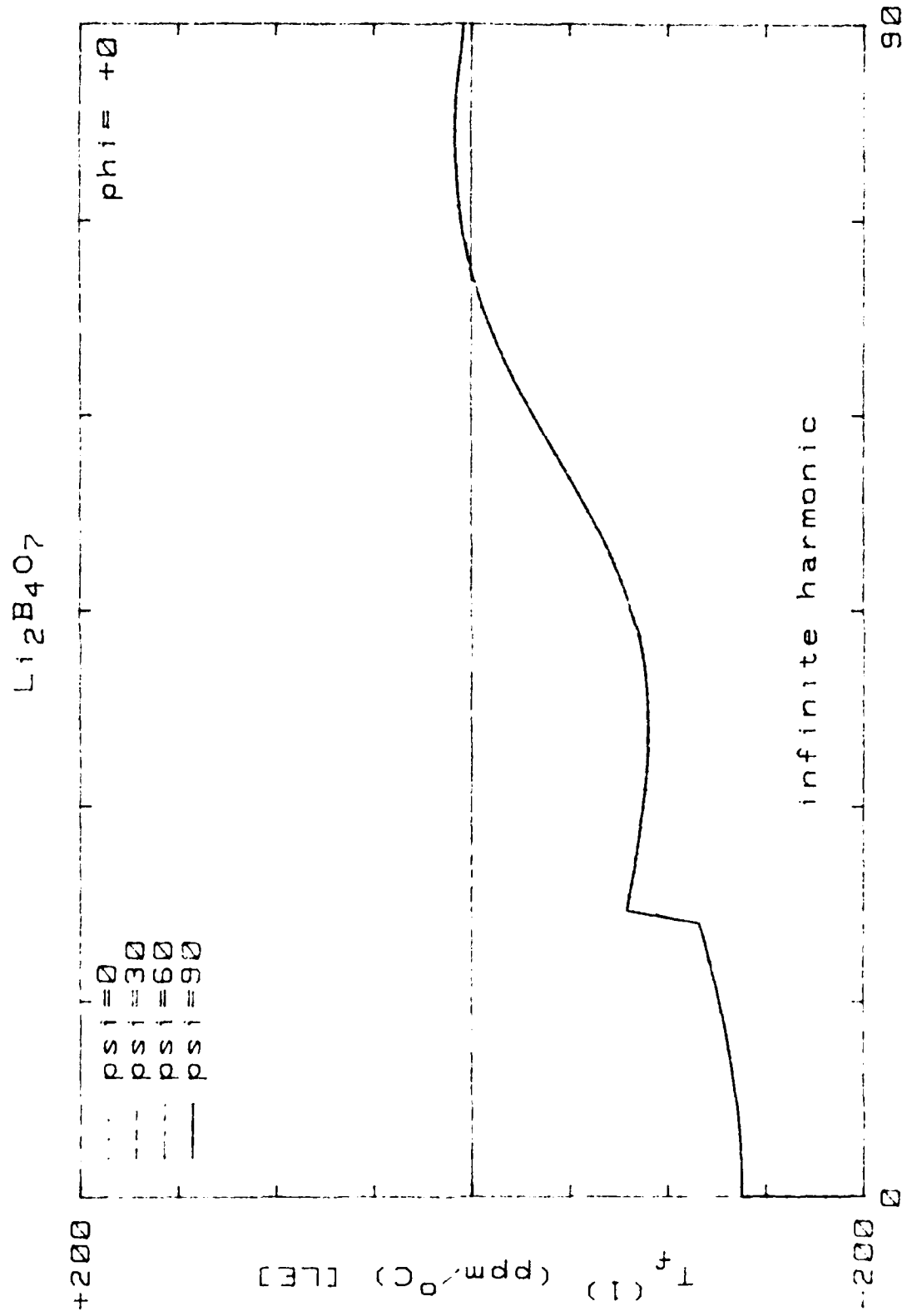

Figure 69. TC(1) for (yxwl)ϕ=0°/θ cuts; M =∞; mode "c"; psi=0°(30°)90°; [LE].

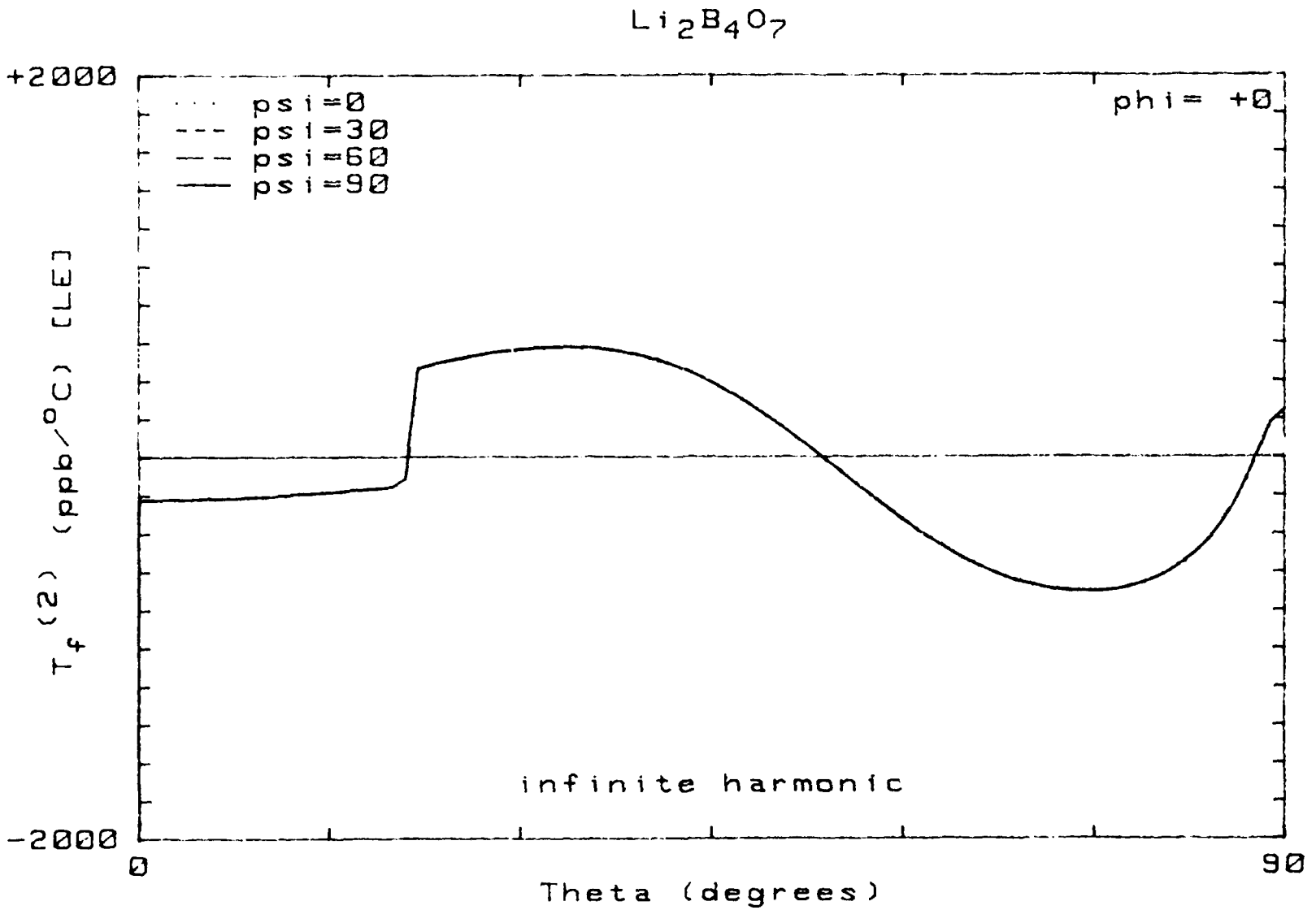

Figure 70. TC(2) for (yxwl)ϕ=0°/θ cuts; M =∞; mode "c"; psi=0°(30°)90°; [LE].

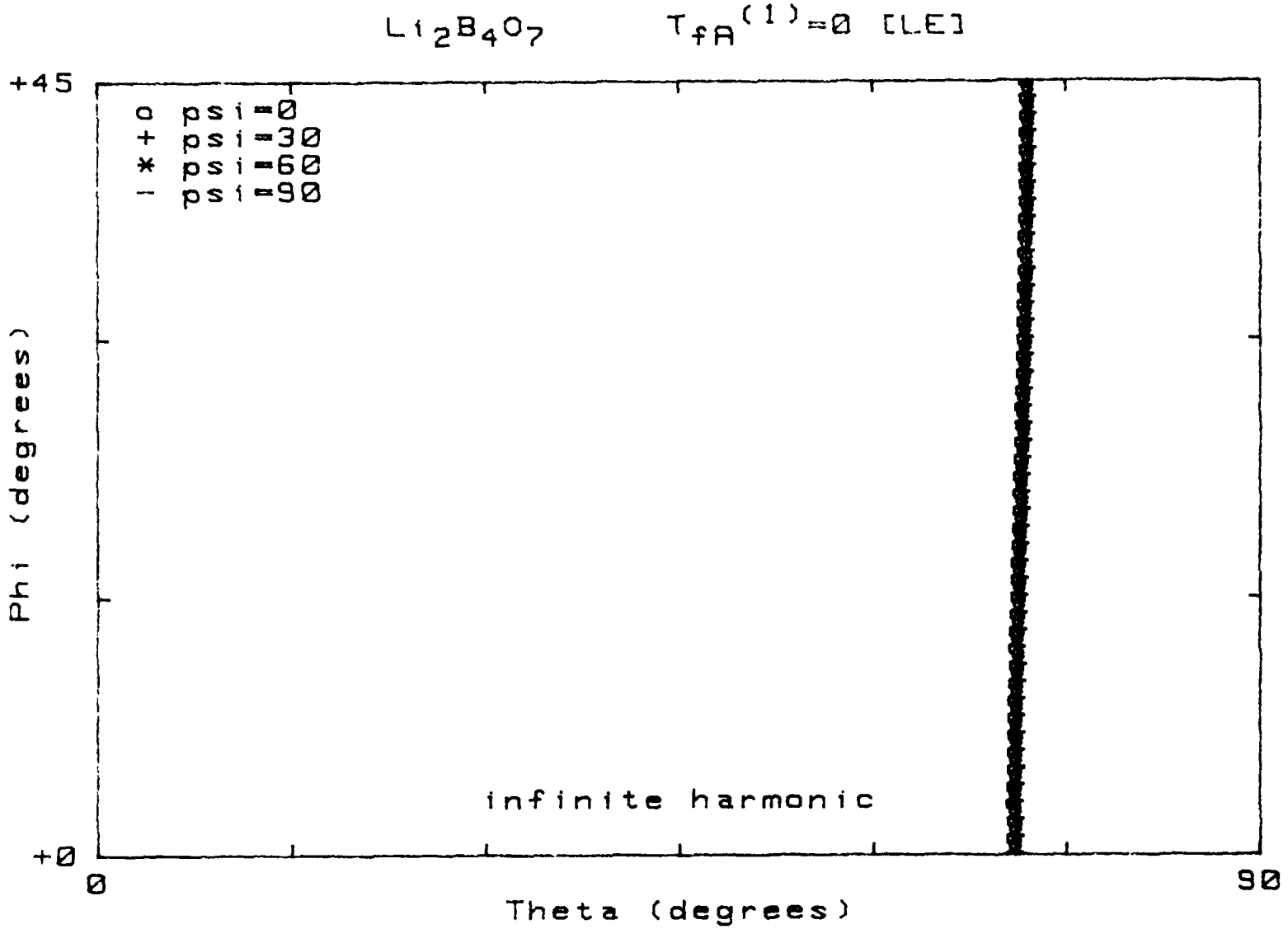

Figure 71. Locus of TC(1)=0 for (yxwl) ϕ /θ cuts; M =∞; mode "c"; psi=0°(30°)90°; [LE].

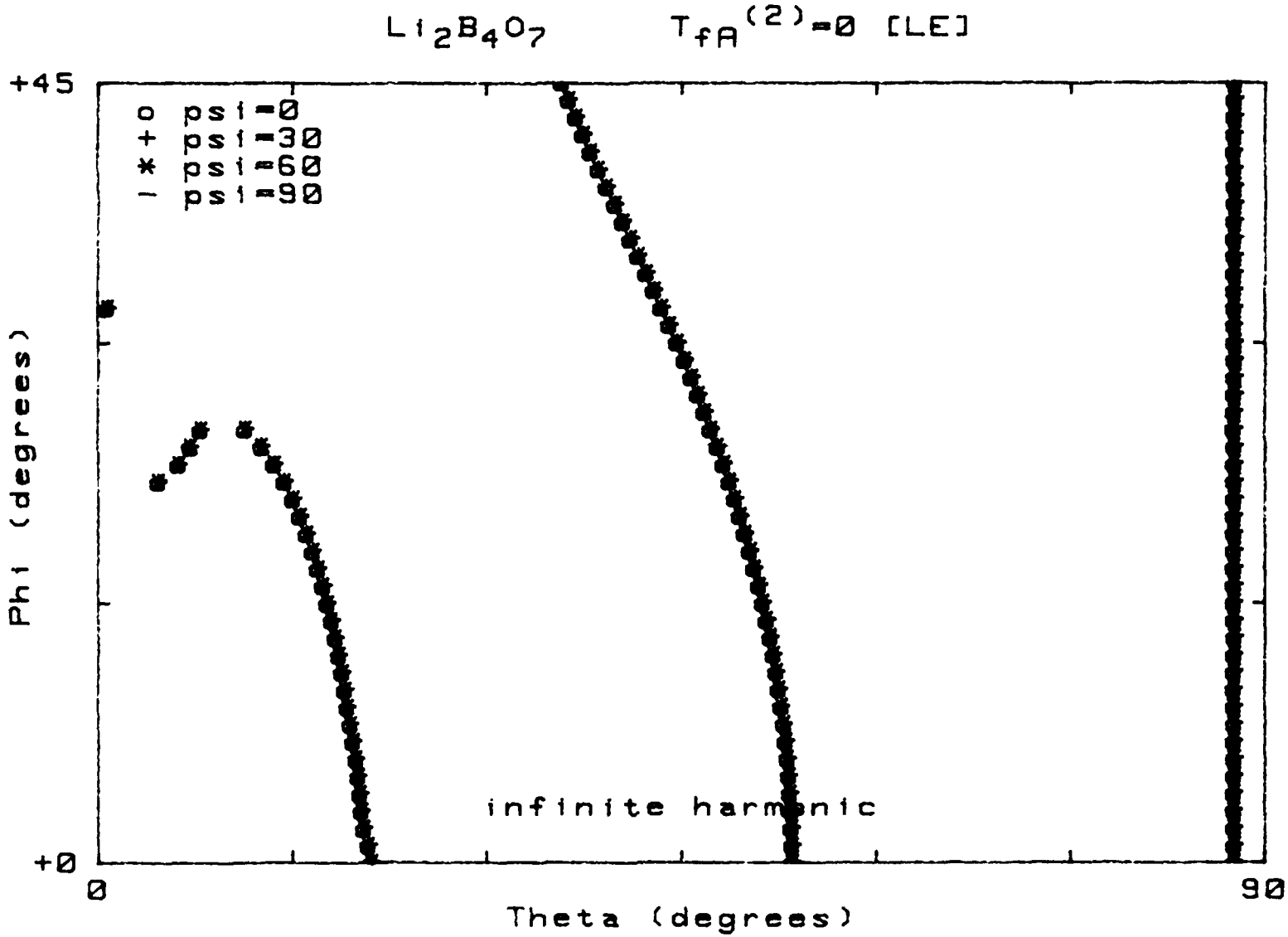

Figure 72. Locus of TC(2)=0 for (yxwl)ϕ/θ cuts; M =∞ ; mode "c"; psi=0°(30°)90°; [LE].

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